APPENDIX B
Comparison/Critique of Exposure Models

This appendix provides a review of several existing and emerging concentration and human exposure assessment models. The review in this chapter is organized according to the general characteristics of the concentration and human exposure models. To begin the review, models were generally classified according to whether they were (1) concentration models or (2) exposure models. Models were then further characterized into more specific categories. For example, the concentration models were further subdivided into outdoor air (Section B.1) and indoor air (Section B.2) concentration models. The exposure models were subdivided according to the exposure media represented: air (Section B.3), consumer products (Section B.4), dietary (Section B.5), and multimedia (Section B.6). Exposure simulation modeling systems were also reviewed (Section B.7). These are not individual models *per se*, rather they are a compilation of various components that are integrated through a common computer system. The parts of this system can include such varied components as air quality models (*e.g.*, atmospheric dispersion models or other types of fate/transport models), Geographic Information System (GIS) capabilities, environmental and various other databases, as well as exposure models and physiologically–based pharmacokinetic (PBPK) models.

This appendix is organized by model categories – air concentration models (*i.e.*, indoor and outdoor air quality models) and human exposure models, therefore facilitating comparison of models with similar characteristics. For the air concentration models (Section B.1 & B.2), "Summary Features" are provided that display the key attributes of each model.

B.1 OUTDOOR AIR CONCENTRATION MODELS

Three models were identified that primarily assess outdoor air concentrations: TOXLT, TOXST, and ASPEN. Both TOXLT and TOXST can be accessed via the EPA's Exposure Models Library (EML) (U.S. EPA 1996c).

B.1.1 TOXLT (Toxic Modeling System Long-Term)

The Toxic Modeling System Long-Term (TOXLT) is a PC-based model that was developed in conjunction with the release of the EPA's Industrial Source Complex (ISC2) Dispersion Models (U.S. EPA 1992b). Both the TOXLT and ISC2 models coincided with the promulgation of the EPA's guidance entitled, "A Tiered Modeling Approach for Assessing the Risks due to Sources of Hazardous Air Pollutants" (U.S. EPA 1992c). The TOXLT computer system was established by OAQPS to examine both the lifetime cancer risks and the chronic noncancer hazard indexes associated with toxic pollutants. The purpose of TOXLT is to assist in the evaluation of the lifetime cancer risks and chronic noncancer hazards that may result from long-term exposure to toxic air pollutants. The ISCLT2 model is used to simulate annual average pollutant concentrations which are then used to estimate cancer risk levels or hazard index values at each user-specified receptor. These outputs presume (1) a hypothetical individual exists at each receptor; (2) no contribution from "background" sources (*i.e.*, sources not specifically included in the simulation); and (3) pollutant contributions in a mixture are additive (*i.e.*, there are no synergistic or antagonistic interactions between pollutants).

Summary Features – TOXLT

Environmental media:	Ambient air
Pollutants:	Multiple gas- and particle-phase agents
Time scale:	Long-term (annual average)
Stochastic:	No
Variability:	No
Uncertainty:	No

B.1.2 TOXST (Toxic Modeling System Short-Term)

The former Integrated Toxic Expected Exceedance Model (INTOXX), which was based on the superseded version of the Industrial Source Complex Short-Term (ISCST) Model, was revised to become the Toxic Modeling System Short-Term (U.S. EPA 1994b). TOXST addresses the problem of estimating expected exceedances of specified short-term health effects thresholds in the vicinity of continuous and intermittent toxic pollutant releases. Certain industrial facilities emit airborne toxic chemicals known to be harmful when their concentrations exceed a specified health effect threshold value for a specified length of time. However, releases of such chemicals often occur intermittently. This random emission pattern makes it difficult to predict the frequency with which ambient concentrations will exceed the health effect threshold. TOXST attempts to avoid the problems of underestimation and overestimation of exceedance rates resulting from random emission patterns by using the Monte Carlo simulation of source emissions of user-specified durations and rates at randomly selected points in time over a simulated long period of time. In addition, TOXST maintains the capability of simulating continuous emission sources along with intermittent emission, thereby providing a more realistic simulation of actual industrial operations.

Summary Features – TOXST

Environmental media:	Ambient air
Pollutants:	Multiple gas- and particle-phase agents
Time scale:	Short term to long-term (~ 1 hour to continuous)
Stochastic:	Yes
Variability:	Yes
Uncertainty:	No

B.1.3 ASPEN (Assessment System for Population Exposure Nationwide)

The Assessment System for Population Exposure Nationwide (ASPEN) was originally developed with support from EPA's Office of Policy (OP) [formally the Office of Policy, Planning, and Evaluation (OPPE)]. The model is being applied by OAQPS as part of their National Air Toxics Assessment (NATA) activities. ASPEN, which is used for hazardous air pollutants, consists of three separate modules (SAI 1999):

1. A dispersion module estimates ambient concentration increments at a set of fixed receptor locations in the vicinity of an emission source;

2. A mapping module interpolates ambient concentration increment estimates from the grid receptors to census tract centroids and sums contributions from all modeled sources; and

3. An exposure module, currently under development, will estimate the average concentration increment to which the population of a census tract is exposed, accounting for time spent in both indoor and outdoor microenvironments and time spent in other census tracts.

The ASPEN dispersion module, like its predecessors HEM and SCREAM2, uses a Gaussian model formulation and climatological data to estimate long-term average concentrations. For each source, the model calculates ground-level concentrations as a function of radial distance and direction from the source for a set of receptors laid out in a radial grid pattern. The concentrations represent the steady-state concentrations that would occur with constant emissions and meteorological parameters. For each grid receptor, concentrations are calculated for each combination of stability class, wind speed, and wind direction. These concentrations are then averaged together. The resulting output of ASPEN's dispersion module is a grid of annual average outdoor concentration estimates for each source/pollutant combination. Improvements to HEM and SCREAM2 that have been incorporated into ASPEN include:

- Expansion of reactive decay options;
- Inclusion of simple treatment of secondary formation;
- Improvement of the deposition algorithm;
- Improved treatment of locations near major point sources; and
- Improved treatment of area and mobile source emissions.

The annual average concentration estimates from ASPEN's dispersion module are then interpolated from the grid receptors to census tract centroids with ASPEN's mapping module. The contributions from all modeled sources are summed to give estimates of cumulative ambient concentration increments in each census tract. The concentration estimates are designed to represent population-weighted concentration averages for each census tract.

The number of emission sources, receptors, and pollutants for an ASPEN application are virtually unlimited. It has been applied to more than 200,000 point, area, and mobile emission sources of 148 hazardous air pollutants to estimate outdoor concentrations in the more than 60,000 census tracts in the contiguous U.S. Work is underway to link an appropriate exposure module to ASPEN.

Summary Features – ASPEN

Environmental media:	Ambient air
Pollutants:	Multiple gas- and particle-phase agents
Time scale:	Long-term (annual average)
Stochastic:	No
Variability:	No
Uncertainty:	No

B.2 INDOOR AIR CONCENTRATION MODELS

Several approaches have been used to estimate expected indoor air pollutant concentrations (for a review, see Wadden and Scheff 1983). These approaches include deterministic models based on a pollutant mass balance around a particular indoor air volume; a variety of empirical approaches based on statistical evaluation of test data and (usually) a least-squares regression analysis; or a combination of both approaches – empirically fitting the parameters of a mass balance model with values statistically derived from experimental measurements. All three approaches have advantages and disadvantages. The mass balance models provide more generality in their application, but often the information on various input parameters is unavailable to carry out a mass balance approach. The empirical models, when applied within the range of measured conditions for which they were fitted, provide more accurate information. Mass balance models include single and multiple compartment models. Often the component of the indoor air mass balance models that is most difficult to represent is the role of indoor surfaces as sources or sinks for pollutants.

B.2.1 INDOOR, EXPOSURE, and RISK (EPA ORD Indoor Air Quality Models)

INDOOR, EXPOSURE, and RISK are a series of three indoor air quality models developed by the Indoor Air/Radon Mitigation Branches of EPA's National Risk Management Research Laboratory within the Office of Research and Development (ORD). The first model, INDOOR, was designed to calculate the indoor pollutant concentrations from indoor sources. The second model, EXPOSURE, extended INDOOR to allow calculation of individual exposure. The RISK model extends EXPOSURE to allow analysis of individual risk to indoor pollutant sources. Risk estimates generated by models such as RISK are useful mainly for the purpose of comparing scenarios, rather than for estimating risks to individuals or populations.

The RISK model uses data on source emissions, room-to-room air flows, air exchange with the outdoors, and indoor sinks to predict concentration-time profiles for all the rooms. The concentration-time profiles are then combined with individual activity patterns to estimate exposure. Risk is calculated using a risk calculation framework. The model allows analysis of the effects of air cleaners located in the central air circulating system and/or individual rooms on IAQ and exposure. The model allows simulation of a wide range of sources including long-term steady state sources, intermittent sources, and decaying sources. Several sources can be modeled in each room. The model allows the analysis of the effects of sinks and sink re-emissions on IAQ. The results of test house experiments were compared with model predictions. The agreement between predicted concentration-time profiles and the test house data was good. The model is designed to run in the Windows operating environment.

Summary Features – INDOOR, EXPOSURE, RISK

Environmental media:	User-specified indoor sources
Pollutants:	Multiple chemicals and radon
Time scale:	Annual average
Stochastic:	No
Variability:	Yes
Uncertainty:	No

B.2.2 MAVRIQ (Model for Analysis of Volatiles and Residential Indoor Air Quality)

The Model for Analysis of Volatiles and Residential Indoor Air Quality (MAVRIQ) (Wilkes et al. 1992) was developed jointly at Carnegie Mellon University and the University of Pittsburgh. It is a compartmental mass balance model that was developed to address human exposure to volatile organic compounds released from showers and other household water uses. In MAVRIQ, the indoor environment is divided into multiple compartments with constant or varying air flows. Based on water supply concentrations as an input, MAVRIQ accounts for pollutant generation, chemistry, and transport kinetics and characteristics of the exposed individual (*i.e.*, water use activity, location, breathing rates).

Summary Features – MAVRIQ

Environmental media:	Ground or surface water
Pollutants:	Volatile organic compounds
Time scale:	Short-term to long-term (~ 1 hour to continuous)
Stochastic:	Yes (but, only for parts of the model)
Variability:	Yes (must be entered repetitively)
Uncertainty:	No

B.2.3 CONTAM (various versions)

The National Institute of Standards and Technology (NIST) has over the past several years developed a series of public domain computer programs for calculating air flow and pollutant dispersal in multi-zone buildings, including CONTAM86, CONTAM87, and CONTAM94. These programs take a multi-zone network approach to airflow analysis. Airflow paths include doorways, small cracks in the building envelope, and a simple model of the air handling system. CONTAM94, the most recent version of CONTAM, works on an Intel®-based PC in the DOS environment. A graphical interface is used to create and edit building descriptions. Future versions of this program are expected to include the capability for carrying out exposure assessments.

Summary Features – CONTAM

Environmental media:	User-specified indoor sources
Pollutants:	Generic
Time scale:	Short term to long-term (~ 1 hour to continuous)
Stochastic:	No
Variability:	No
Uncertainty:	No

B.2.4 AMEM (ADL Migration Exposure Model)

The ADL Migration Exposure Model was developed by EPA's Office of Pollution Prevention and Toxics (OPPT) to estimate the migration of chemicals from polymeric materials such as television cabinets, water pipes, curtain backings, plastic toys, or other products containing polymers in home environments where these chemicals could become sources of indoor air pollution or contaminate potable water. Once the fraction of chemical that can migrate from a product is estimated, external models can be used to estimate the exposures and risk to people from contaminated indoor air or water. The AMEM provides estimates for screening-level assessments when data are not available. The goal of the model is to identify concentrations that result in possible health concerns to justify further emission testing of the product for polymeric materials.

Summary Features – AMEM

Environmental media:	Indoor environment
Pollutants:	Chemicals emitted by polmeric materials
Time scale:	Short term
Stochastic:	No
Variability:	No
Uncertainty:	No

B.3 HUMAN INHALATION EXPOSURE MODELS

Most human exposure models have the capability to track humans, either as individuals or in groups (*i.e.*, cohorts[1]) through their daily routines. The tracking process includes knowing where the person is, what they are doing (*i.e.*, their activities, including knowledge of the physical demand that the person is exerting during an activity), and the concentration of the pollutants that they come into contact with as they move about.

With the knowledge that outdoor air pollutants are able to penetrate into the interior of buildings and that many air pollutants are emitted by both outdoor and indoor sources, a great deal of work has focused on combining the features of both indoor and outdoor exposure models. These models differ in their approach, but all of them estimate exposures to outdoor pollutants that penetrate into buildings. The building type of greatest concern for estimating indoor exposures is probably residential buildings. A national study on human activities found that on average, U.S. citizens spend 69 percent of their time indoors at home (U.S. EPA 1996a). This percentage can be higher for some subsets of the population; for example, the very young or the elderly. Therefore, it is important to be able to model the pollutants of concern to human health that can penetrate a building's structure. The models in this section have, through various techniques, attempted to develop an integrated assessment of the exposure mechanisms associated with airborne pollutants from both indoor and outdoor sources. Descriptions of the models are provided below.

B.3.1 NEM and pNEM [The (probabilistic) National Ambient Air Quality Standards Exposure Models]

The EPA has used the NEM modeling methodology since the late 1970s when three pollutant-specific versions of the NAAQS Exposure Model (NEM) were developed for ozone (O_3), carbon monoxide (CO), and particulate matter. The early versions of the NEM were referred to as "deterministic" as they did not attempt to model the random processes of people's activities as part of the exposure simulation. The models simulate the movements of specific subgroups or cohorts within a population through zones of varying air quality. Each zone is typically defined by a geographic location and a microenvironment. The movements of each cohort are determined by the use of activity diary data specific to the demographic characteristics of the cohort. The activity data are also specific to day of the week, season, and temperature. Depending on the application, cohort movements may account for trips to work places or to schools.

From its inception,NEM was designed to treat human exposure to airborne pollutants as a time series of a joint set of human activities occurring in a particular microenvironment and air quality (as measured by the concentration of a pollutant) in that same microenvironment. Maintaining the time series allows estimates for alternative exposure and dose metrics to be developed, a capability that has proven invaluable (McCurdy 1997).

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[1] A cohort is comprised of persons with similar demographic characteristics. A cohort is defined by a specific combination of home district (where they reside), work district (their place of employment), and demographic variables (*e.g.*, gender, age).

In 1988, the Monte Carlo technique for randomly selecting important variables was incorporated into the model simulations. These models were referred to as "probabilistic" and hence are known as probabilistic NEM, or pNEM. The models are pollutant specific. To identify one version of the model from another, the chemical symbol is appended to the pNEM-acronym; hence, the model for ozone is pNEM/O_3 and for carbon monoxide is pNEM/CO. These two models are the most commonly used pNEM models today. Developing the probabilistic versions of the model was an important step because it meant that the entire distribution of available data for each variable in a model could now be used. This makes it easier to address variability and uncertainty regarding the variables that were in the model (McCurdy 1997).

The first pNEM developed was that for ozone, or pNEM/O_3. The early pNEM/O_3 used a regression-based relationship to estimate indoor concentrations of ozone using concentrations measured outdoors. Then, in 1991, a new version of pNEM applicable to carbon monoxide (pNEM/CO) was developed (Johnson et al. 1992b). This model was the first to use a mass balance model to estimate indoor pollutant concentrations. The mass balance model is based on the generalized mass balance model presented by Nagda et al. (1987). In general terms, the mass balance model can be described as:

The change in indoor pollution concentration =
the pollutant entering from outside
+ the indoor generation of pollutant
— pollutant leaving the indoor microenvironment
— removal of the pollutant by an air cleaning device
— decay of the pollutant indoors.

Another version of the pNEM/O_3 soon followed which also used a mass balance model to estimate indoor ozone concentrations. Several other refinements were included in this new version of the pNEM/O_3. Some of these include the use of more recent census data for determining demographic information, a new commuting algorithm, and an increase in the number of fixed-site monitors able to represent each urban area.

Early in 1994, a special version of pNEM/O_3 applicable to outdoor workers was developed and used to estimate ozone exposures for outdoor workers in several cities in the U.S. (Johnson et al. 1996c). In a follow-up effort, another version of pNEM/O_3 specific to children who were active in outdoor activities was developed (Johnson et al. 1996c).

More recently, enhancements have been completed on the pNEM/CO. The latest version of the model is pNEM/CO (Version 2.0). Improvements to this model include the use of an expanded human activity database. This database is called the Comprehensive Human Activity Database (CHAD) (McCurdy 1999). The CHAD is comprised of over 17,000 person-days of activity pattern data. The data have been collected and organized from eight human activity pattern surveys. The CHAD contains the sequential patterns of activities for each individual, which is particularly important to estimating the dose profile for CO by the model. Another enhancement to pNEM/CO (Version 2.0) is the inclusion of a special commuting database developed by the Bureau the model for creating an "origin-destination" table to indicate the patterns of commuting trips made by working cohorts among the defined exposure districts (Johnson et al. 1999).

Improvements have been made to both the algorithms and inputs to the mass balance model in pNEM/CO (ver. 2.0). The pNEM/CO methodology includes a mass balance model, which is used to estimate CO concentrations when a cohort is assigned to an indoor or motor vehicle microenvironment. The mass balance model is based on the generalized mass balance model presented by Nagda et al. (1987). As originally proposed, this model assumed that pollutant concentration decays indoors at a constant rate. For use in pNEM/CO, the Nagda model was revised to incorporate an alternative assumption that the indoor decay rate is proportional to the indoor concentration (Johnson et al. 1999). This alternative assumption is believed to more closely model the actual decay rate that takes place indoors. In addition, new databases and improved algorithms have been included for determining air exchange rates, the probability of gas stove use, gas stove-burner emission rates, pilot light emission rates, and residential volumes used in the mass balance model (Johnson et al. 1999).

The pNEM/O_3 and pNEM/CO are part of a small group of exposure models in which attempts have been made to evaluate their results using personal exposure monitoring data. Johnson et al. (1996c) describes initial efforts to evaluate the pNEM/O_3. In this effort, pNEM/O_3 exposure estimates for Houston, Texas were compared with personal exposure monitoring data collected in 1981 during the Houston Asthmatic Study (HAS) (Stock et al. 1985). A special version of the pNEM/O_3 was created, which corresponded to the data collection criteria for the HAS. Results were compared for distributions of both one-hour ozone exposure estimates and one-hour daily maximum ozone exposure estimates. In general, the results suggested that the model overpredicted the HAS exposures in the range below 70 ppb and underpredicted exposures above 70 ppb. Developers of the pNEM/O_3 believed that the exposure estimates of the model were particularly sensitive to the distribution of ozone decay rates used in the model's mass balance algorithm (Johnson et al. 1996c).

During early model development, the execution of the pNEM series of models was conducted only on an EPA mainframe computer because of the large input and output data files required to run the model. However, in the summer of 1999, pNEM/CO (Version 2.0) was migrated (that is transferred) to run on a PC. OAQPS and ORD's NERL are continuing to support efforts to improve the efficiency of pNEM on a PC and to provide documentation and user's guides for the PC version. The documentation and code for the PC version of pNEM/CO should be available for public release in 2000.

The pNEM/CO (Version 1) was evaluated using CO exposure data collected during the Denver Personal Exposure Monitoring Study conducted during the winter of 1982/83 (Akland et al. 1985). Researchers analyzed the Denver data to determine the one-hour daily maximum and the 8-hour daily maximum CO exposures associated with each person-day of data. Then, the pNEM/CO was run to simulate the conditions of the Denver Personal Exposure Monitoring Study. The exposure estimates from this application were tabulated according to the classification of each cohort with respect to the type of cooking fuel used (*i.e.*, natural gas or other). The researchers found relatively good agreement between the observed and estimated distributions for the one-hour daily maximum analyses, except for the values above the 99^{th}

percentile. They did not find as good agreement between the observed and estimated distributions for the eight-hour daily maximum exposures. The researchers reported that in each case, the distribution obtained from pNEM/CO overestimated the exposure values at low exposures and underestimated the exposure values at high exposures. The researchers point out that the estimated and observed distributions for the eight-hour daily maximum exposures agreed most closely in the range of CO concentrations between 5 and 12 ppm (Johnson et al. 1992b).

The pNEM/CO (Version 1) was evaluated similarly to the Johnson et al. (1992b) evaluation effort but with the additional use of the Kolmogorov-Smirnov test statistic to compare the observed and simulated cumulative frequency distributions for the one-hour daily maximum exposure (1DME) and the eight-hour daily maximum moving average exposure (8DME) (Law et al. 1997). A similar effect to that seen in the evaluation of the pNEM/O_3 occurred for pNEM/CO. For 1DME, the pNEM/CO exposure estimates agreed most closely with observed exposures within the middle of the distribution; that is, in the range of approximately 6 to 13 ppm. However, the model overestimated values at low exposures (*i.e.*, less than 6 ppm) and underestimated values at high exposures (*i.e.*, greater than 13 ppm). For 8DME, the estimated exposures agreed well with observed exposures in the range of CO concentrations between about 5.5 and 7 ppm. However, the model overestimated values below 5.5 ppm and underestimated values above 7 ppm (Law et al. 1997).

B.3.2 HAPEM (The Hazardous Air Pollutant Exposure Model)

In 1985, the EPA's Office of Mobile Sources (OMS) developed a model for estimating human exposure to nonreactive pollutants emitted by mobile sources. This model is similar to the pNEM in that it simulated the movements of population groups between home and work locations and through various microenvironments. However, they differed in the temporal resolution used for expressing the exposure estimates. The pNEM provided hourly exposure estimates which could be averaged over longer time periods, whereas the HAPEM provided annual average exposure estimates. The HAPEM included a facility for estimating cancer incidence through the use of risk factors developed by the EPA, but the pNEM does not include this capability.

Then, in 1991, OMS extended this modeling methodology to estimate annual average carbon monoxide (CO) exposures in urban and rural areas under specified control scenarios. The model was now called the Hazardous Air Pollutant Exposure Model for Mobile Sources (HAPEM-MS). The annual average CO exposures could be used to estimate annual average exposures to various hazardous air pollutants associated with mobile sources. In each case, it was necessary to assume that the annual average exposure to a particular hazardous air pollutant was linearly proportional to the annual average CO exposure. The model was executed for specified urban areas that had ambient fixed- te CO monitors.

Shortly after, under the direction of EPA's Office of Research and Development (ORD), an enhanced version of the HAPEM-MS was developed. This model was labeled the HAPEM-MS2. It sub-divided the annual exposures by calendar quarter (*i.e.*, 3-month periods) to better estimate exposures to mobile sources as a consequence of outdoor air temperature. The HAPEM-MS2 also increased the number of microenvironments to 37, increased the number of demographic groups[2] to 23, and increased the size of the activity pattern database (Johnson et al. 1993a).

In 1996, the EPA's ORD further enhanced the HAPEM by creating another generation of the model called the HAPEM-MS3. The enhancements included adding the ability to customize the demographic groups, updating the census data by using the 1990 census, and developing an algorithm for estimating ambient impacts in residences with attached garages (Palma et al. 1996).

Until the spring of 1998, execution of the HAPEM-MS3 operated only on an EPA mainframe computer. During early model development, this limitation was necessary as the model requires large data files for storage and large internal arrays for calculation. Then, by 1998, with advances in computing technology, it became possible to have the HAPEM-MS3 executed on a "workstation." To this end, in the spring of 1998, the HAPEM-MS3 was migrated (that is transferred) to the UNIX operating system on a workstation. During the migration, further enhancements to the model were made, including a new time-activity database derived from the CHAD, a new air quality program that automatically selects sites, and a more efficient implementation of the commuting algorithm.

Immediately after the release of the UNIX-version of the HAPEM-MS3, the ORD again made substantial improvements to the model. The newest model had two distinct improvements over the 1998 UNIX-version. First, the areal extent of the model was expanded to include the entire contiguous United States at the census tract-level. In order to make this possible, the second innovation to the model was the facility to use modeled air quality data as well as AIRS data. With this improvement, the model for the first time was able to *directly* estimate exposures to hazardous air pollutants; hence, the model was renamed again by dropping the mobile source (-MS) acronym. This latest version of the model, called the HAPEM4, has other enhancements as well. These include broader flexibility in defining the study area (this can range from a census tract up to the entire contiguous U.S.), an updated database of temperatures, an updated commuting algorithm, population data for all census tracts in the country, and the ability to change internal modeling parameters such as the number of microenvironments and the demographic group designations.

B.3.3 HAPEM-PS (The Hazardous Air Pollutant Exposure Model for Point Sources)

The Hazardous Air Pollutant Exposure Model for Point Sources (HAPEM-PS) was initially developed for OAQPS. In its original form, HAPEM-PS was intended to be applied to factories, refineries, and other stationary point emission sources. The HAPEM-PS requires an air quality indicator (*e.g.*, annual mean concentration) for each point in a receptor grid surrounding the point source under evaluation. Receptor air quality values are typically determined through the use of emissions data and a dispersion model. The HAPEM-PS has not had the same extensive enhancements that the HAPEM-MS has had since the early 1990s.

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[2] A demographic group is defined by specific demographic characteristics taken from the census. For example, in HAPEM demographic groups are typically defined by gender, age, race, and working status (*i.e.*, either working or non-working).

Like the HAPEM-MS, HAPEM-PS defines exposures for sets of cohorts. However, the population of concern in HAPEM-PS is usually defined as all persons residing within a specified distance from a particular emission source. The pollutant concentrations at the receptors are typically estimated by the ISCLT dispersion model. Input data for the ISCLT model include local meteorological data and an estimate of the pollutant emissions from the source. In a typical HAPEM-PS application, the ISCLT model is used to estimate the annual average pollutant concentrations at the centroid of each of the census units used to define the home and work districts and at regularly-spaced receptors along the emission source property line. The HAPEM-PS output provides a histogram of the total number of people exposed at pollutant concentration level intervals. The HAPEM-PS output also provides the annual cancer incidence by home district, the home district population, and the cancer incidence per million individuals for each home district. Finally, the output includes the value and cohort of the maximum exposure and the values and home districts of the maximum lifetime cancer incidence and incidence rate (Johnson et al. 1993b).

B.3.4 AirPEx (Air Pollution Exposure Model)

The AirPEx was developed at the National Institute of Public Health and the Environment in the Netherlands as a tool for analyzing the inhalation exposures of the Dutch population to air pollutants. The model was designed to assess and evaluate the time- and space-dependency of inhalation exposures of humans. It can be used to evaluate individuals, as well as populations and subpopulations.

The AirPEx estimates personal exposure for one-hour time intervals. The exposure parameters calculated include (1) the potential exposure concentrations (the air concentration as a function of time and space (*i.e.*, microenvironments)), (2) the actual exposure concentration (the concentration that a person moving through the microenvironment experiences as a function of time, (3) the intake rate (the rate at which a pollutant enters the respiratory tract per unit time, (4) the standardized intake rate (the intake rate standardized to the target organ (*e.g.*, lung, body mass), (5) the frequency and time fraction that a person is in contact with concentrations above a certain threshold value, (6) the critical intake (the excess intake at exposure concentrations above critical concentrations) (Freijer et al. 1997). Averages for each of these variables can be obtained for an exposure period by integrating them over the whole period and dividing by the time span of the period.

Population exposures are approximated by repeating individual calculations for a large sample of individuals taken randomly from the whole population. The distribution of the calculated individual average exposures are approximated for the whole population by the probability density function. Analysis of the distribution in terms of percentiles yields information on the median, and extremes in the exposure levels are quantified by the 10th and 90th percentiles (Freijer et al. 1997).

The model itself consists of three modules assembled in the Windows® environment. The program retrieves data from two databases and uses numerous compound specific parameters. Default values for benzene, B(a)P, ozone, and PM are included in the program. Users can override the default values and supply their own values for these four compounds, as well as for other compounds. The main module calculates individual exposure measures from time-series of air quality data and human activity patterns. Exposures are estimated in 15-minute discrete time-steps for various microenvironments. The AirPEx currently uses a database containing 4,985 daily activity patterns with 15-minute time resolution for the population in the Netherlands. Time series of air quality are supplied with one-hr resolution. A second module selects records from the activity pattern database. It estimates population exposures by repeating individual exposure calculations for all selected activity patterns and then combining this information to construct normalized frequency distributions. A third module displays the results of the exposure calculations and analyzes the distributions by percentiles. An important feature is the ability to analyze the socioeconomic characteristics of the individuals having the highest exposures to enable identification of high risk groups.

B.3.5 HEM (Human Exposure Model)

In 1980, the EPA's OAQPS developed the Human Exposure Model (HEM). The model was designed to screen point sources of air pollutant emissions efficiently, ranking the sources according to their potential cancer risks. Then, in 1990, an updated version (HEM-II) that had additional modeling capabilities needed to address issues related to the analysis of toxic air pollutants was released. The HEM-II was intended for use in evaluating potential human exposure and risks from sources of toxic air pollutants (U.S. EPA 1991). HEM-II retained the capability of screening point sources for a single pollutant in order to rank sources according to cancer risks. The HEM-II also allows more refined analyses of individual point sources and study of entire urban areas that include multiple point sources, multiple pollutants, area sources, and dense population distributions.

The HEM-II uses the Industrial Source Complex Long-Term (ISCLT) Model for estimating dispersion. The HEM-II also provides the ability of moving the exposed population into up to ten microenvironments. These may include indoors at home, indoors at work, in transit, and movement out of the study area. For each application, parameters can be defined for indoor-outdoor concentration ratios for each microenvironment, the percentage of the exposed population to be assigned to the microenvironment, and the amount of time, on an annual basis, estimated to be spent in each microenvironment. New to this revised version of the model is the quantification of several key uncertainties. Using the Monte Carlo technique, six input variables can be described by distributions. They are the unit risk factor, the emission rate, microenvironmental concentrations, the time spent in a microenvironment, years spent in current residence, and the variability in concentrations predicted at the receptors. A choice of several statistical distributions can be selected for each input variable.

The HEM-II contains a limited STability ARray (STAR) database within the model. Complex emissions inventories can also be modeled. This includes modeling area sources (*e.g.*, mobile sources, residential heating) simultaneously with point sources. A choice of grid systems, including a Cartesian grid that will accommodate areas with high population density and numerous air pollution sources, is offered for calculating exposures. Population growth can be simulated, either from the base year of the population database to the current year or to a future year. The model allows the user to account for differences between microenvironments (*i.e.*, indoor and outdoor concentrations). Census coverages are for the entire U.S. at the block group level. The results of the model's output can be shown graphically.

B.3.6 SHAPE (Simulation of Human Activities and Pollutant Exposure)

EPA's ORD developed the Simulation of Human Activities and Pollutant Exposure (SHAPE) (Ott et al. 1988). SHAPE generates carbon monoxide inhalation exposure profiles for different human subgroups. It considers exposure to carbon monoxide in air through the inhalation pathway only. The model has two major input components: (1) human location patterns, and (2) microenvironmental carbon monoxide concentrations. It matches available location/activity data with environmental concentration data to obtain exposure profiles for 24-hour periods. Exposure concentrations are obtained by applying a superposition principle to contributions from the ambient and different microenvironments. In addition to the limited evaluations conducted on pNEM, SHAPE is one of the only other exposure models where attempts were made to evaluate the model's estimates using personal exposure data. The EPA's Denver/Washington, D.C. personal exposure database was used to test the model's predictions against 24-hour exposure profiles for more than 1,200 persons (Ott et al. 1988).

B.3.7 BEAM (Benzene Exposure Assessment Model)

The Benzene Exposure Assessment Model's (BEAM) initial development by EPA's ORD in the late 1980s was spurred, at least in part, as a result of benzene being listed as a hazardous air pollutant by the Clean Air Act and because benzene is regarded as a human carcinogen (U.S. EPA 1990a). The model utilizes microenvironmental benzene concentration data coupled with human activity pattern data to estimate exposure to benzene. The BEAM estimates benzene inhalation exposure profiles for different human subgroups. It considers exposure to benzene in air through the inhalation pathway only. The model has three major input components: 1) human location patterns, 2) ambient (background) benzene concentrations, and 3) microenvironmental benzene concentrations. It matches available location/activity data with environmental concentration data to obtain exposure profiles for 24-hour periods. Exposure concentrations are obtained by applying a superposition principle to contributions from the ambient and different microenvironments. Inhalation dose is then obtained by applying inhalation rate to exposure concentrations. The BEAM was patterned after the Simulation of Human Air Pollution Exposure (SHAPE) model.

The Total Exposure Assessment Methodology (TEAM) studies conducted between 1979 and 1988 by the U.S. EPA have been cited as providing the impetus for developing a human exposure assessment model for benzene. The TEAM studies strongly indicated that human exposure to certain classes of volatile organic compounds (VOC), including benzene, occurs primarily within the confines of very restrictive microenvironments, primarily indoors, but outdoors as well. The TEAM studies also suggested that the traditional method of estimating exposures to benzene (as well as most VOCs) did not adequately account for the contribution of benzene from small, nearby sources. Therefore, the developers of the BEAM endeavored to develop an exposure simulation model for benzene that utilized microenvironmental benzene concentrations data coupled with human activity pattern data to estimate human exposure to benzene (U.S. EPA 1990a, U.S. EPA 1993a). The BEAM is one of the models included in EPA's THERdbASE (see Section B.7.2).

B.3.8 pHAP (probabilistic Hazardous Air Pollutant exposure model)

The probabilistic Hazardous Air Pollutant (pHAP) exposure model was developed by the EPA to estimate exposures to HAPs for the population residing in a specified study area. The model uses census data, ambient air quality data, meteorological data, and human activity pattern data to simulate exposures to the population from several different HAPs. The original version of the pHAP model was developed for a mainframe computing system. The mainframe version was developed and used to estimate benzene exposures to residents of a study area in Phoenix, Arizona for the year 1990. Subsequent to that development, a PC-version of the model was developed and tested using the same study area. The PC-version of the model is called, pHAP-PC. The pHAP-PC model utilizes a Graphical User Interface (GUI) to provide a Windows®-like environment (Panguluri et al. 1998).

B.3.9 CPIEM (California Population Indoor Exposure Model)

The California Population Indoor Exposure Model was developed for the California Air Resources Board's (ARB) Indoor Program to evaluate indoor exposures for the general California population as well as certain subgroups such as individuals who may be highly sensitive to indoor air pollutants. The ARB required a model which could estimate the average and peak indoor exposures for the population and sensitive subgroups. The CPIEM combines indoor air concentration distributions with Californians' location and activity information to produce exposure and dose distributions for different types of indoor environments. This task is achieved through a Monte Carlo simulation whereby a number of location/activity profiles that were collected in ARB studies are combined with airborne pollutant concentrations for specific types of microenvironments (*e.g.*, residences, office buildings).

Concentration distributions for many pollutants and microenvironments are included in the CPIEM database. However, for pollutants and microenvironments not included in the database, the CPIEM presents two alternatives. The first is to estimate indoor air concentration distributions based on distributional information for mass balance parameters described below. The second is for the user to directly specify concentration distributions. The concentration values for a particular environment are then sampled from the distributions.

The simulation of indoor concentrations accounts for various types of indoor sources as well as outdoor concentrations, air exchange rates, and losses to indoor sinks. The concentration component (called a module) of the model uses a mass balance equation, based on the principle of conservation of mass, to estimate concentration distributions for specific types of indoor environments such as residences, offices, and schools. This module samples values from user-specified distributions for parameters such as emission rates for indoor sources, building volumes, outdoor air concentrations, and indoor-outdoor air exchange rates, which are used as inputs to the mass balance equation.

Multiplication of the concentration values by breathing rates determined from the location/activity profiles and pulmonary ventilation data yields an estimate of the potential inhaled dose distribution for each modeled environment. The model then aggregates the environment-specific exposure and dose estimates to develop distributions of "total indoor air" exposures and doses. That is, the portion of the total (24 hour) exposure/dose associated with time spent indoors. Because outdoors are included as one of the environments in the model, it is also possible to simulate the total (both indoor and outdoor) exposure and dose distributions (CARB 1998).

B.4 CONSUMER PRODUCT EXPOSURE MODELS

A few exposure models have been developed to assess potential exposures associated with the use of household consumer products. This type of exposure model is not as numerous as those found in the previous three sections because these models deal solely with pollutants emitted by the consumer products. The emissions from these products occurs primarily indoors where relatively few regulations exist for controlling toxic emissions. However, unlike the exposure models in the previous section that estimated exposures exclusively by the inhalation route, two of the models in this section can also estimate exposures by ingestion and/or dermal contact.

B.4.1 CONSEXPO (CONSumer EXPOsure Model)

The CONSumer product EXPOsure model (CONSEXPO) (Van Veen 1995) developed by the National Institute of Public Health and the Environment (RIVM) [Netherlands] uses simple exposure and uptake models to assess the potential health impacts of consumer products. In order to cope with the diversity in consumer products, it is based on a general model framework that provides a general setting for widely differing exposure situations, and, secondly, it offers a number of predefined exposure/uptake models, which the user can link to build a complete exposure/uptake model. The starting points are the inhalation, dermal, and ingestion exposure pathways. For each of these pathways, a limited number of models is available to model exposure/uptake. The program reports several important exposure variables, namely, the per event concentration, the yearly averaged concentration, the fraction taken up, the amount taken up during a year (per year and summed), and the uptake per kilogram body weight per day. The program also allows for stochastic parameters, in order to propagate the effects of variable and/or uncertain parameters to the final exposure/uptake estimates. If one uses the stochastic parameters, the resultant distributions can be displayed and studied.

B.4.2 SCIES (Screening Consumer Inhalation Exposure Software)

The Screening Consumer Inhalation Exposure Software (SCIES) was developed to assist the Economics, Exposure, and Technology Division of U.S. EPA's Office of Pollution Prevention and Toxics in performing screening-level assessments of the potential dose rates resulting from inhalation of new and existing chemicals in consumer products. The model calculates screening-level estimates of average individual inhalation potential dose rates to components of consumer products that can be classified into 11 different product categories. The model estimates potential dose rates for both actively-exposed users of the product and passively-exposed non-users. Default values are suggested for each parameter required to run the model for each product category. These values are based on exposure scenarios, volatility classifications, and residence occupancy patterns. The model combines results of an effort to measure ventilation flows within residences with a 2-zone mass balance model to allow estimation of potential dose rates to both consumer product users and non-users.

B.4.3 DERMAL

DERMAL was developed to assist the Economics, Exposure, and Technology Division of U.S. EPA's Office of Pollution Prevention and Toxics in performing screening-level assessments of the potential dose rates resulting from dermal contact with consumer products containing new and existing chemicals in consumer products. The model calculates screening-level estimates of annual individual dermal potential dose rates to components of 16 consumer product categories. Exposures are calculated based on the weight fraction of the chemical of interest in the consumer product and assuming deposition of a film of liquid on to the dermal surface from contact with the product. Conservative default values are provided for most of the input parameters required to run the model for each of the 16 consumer product categories.

B.4.4 MCCEM (Multi-Chamber Concentration and Exposure Model)

The MCCEM is an interactive model developed for the EPA's OPPT and updated for the EPA's ORD. It allows users to model indoor air contamination for use in assessing potential inhalation exposures caused by consumer products. The objective of MCCEM is to allow users to be able to assess the risk from exposure to pollutants emitted by consumer products. The model uses a spreadsheet format to estimate indoor concentrations for, and individual exposures to, chemicals released from products in residences. Concentrations can be modeled in as many as four zones within a house. The model can supply air exchange rates and interzonal airflows for different types of residences. Time-varying emission rates can be input for a pollutant in each zone of the residence, for outdoor concentrations, and for the zone where an individual is located. In this way, the model develops a time-series exposure profile for the individual.

The MCCEM allows the user to explore the sensitivity of the model results to changes in one or more of the input parameters. The parameters that can be modified in the sensitivity analysis include the infiltration rate, the source rate, the decay rate, and the outdoor concentration.

B.5 DIETARY EXPOSURE MODELS

B.5.1 DEPM (Dietary Exposure Potential Model)

The Dietary Exposure Model (DEPM) is a model and database system developed by U.S. EPA's ORD to correlate food information in a format for dietary exposure modeling. Currently, the database system includes information from several national, government-sponsored surveys and monitoring programs. In the model, food consumption is based on 11 food groups, containing approximately 800 core food types, established from over 6500 common food items. A unique feature of the DEPM is the use of recipes, developed for exposure analysis, that link consumption survey data to the pollutant residue information. The summary databases are aggregated in a fashion to allow the analyst selection of demographic factors, such as age/sex groups, geographical regions, ethnic groups and economic status. The model was developed for personal computers with the data files designed in dBASE IV with FoxPro for Windows applications programs for queries and reporting.

B.6 MULTIMEDIA EXPOSURE MODELS

This section presents a review of a number of multimedia models that address exposure links among multiple ambient environmental media and multiple exposure media.

B.6.1 The Exposure Commitment Method

One of the earliest approaches for systematically assessing multipathway exposures to environmental pollutants is termed the Exposure Commitment Method, developed by Bennett (1981). The basic objective of this approach is to calculate exposure commitments (*i.e.*, pollutant concentration in human tissue), which are calculated from transfer factors that are estimated as the ratios of the steady-state concentrations of a pollutant in adjoining compartments of an exposure pathway. An exposure commitment is determined by multiplying the transfer factors associated with the adjoining compartments of a given pathway of exposure, for example; air to plants to livestock to diet. This method has been applied to organic chemicals and metals. The published applications of the exposure commitment methodology depend on measured concentrations of the substances in different compartments to estimate transfer factors. The retrospective nature of this approach limits its usefulness for predicting exposures to chemicals for which there is little or no monitoring data available.

B.6.2 Layton et al. (1992) Indoor/Outdoor Air/Soil Transport Model

In recent years various researchers have begun to model algorithms that address the movement of fine and coarse particles in the indoor environment by processes such as resuspension, deposition, and soil tracking (see Raunemaa et al. 1989; Nazaroff and Cass 1989; Allott et al. 1992). Nevertheless, none of these algorithms provide an integrated simulation of major transport processes and indoor/outdoor relationships for toxic substances in air, water and soil. In order to estimate concentrations of pollutants in the media identified here, one needs an indoor transport model that simulates (1) the movement of pollutants from the outdoor environment (air and soils) to the indoor environment and (2) the resulting concentrations in indoor media (air and floor dusts) resulting from both outdoor and indoor sources of the target pollutants.

Layton et al. (1992) have developed for particle bound radio nuclides a pollutant transport model that accounts for (1) the movement of pollutants from the outdoor environment (air and soils) to the indoor environment and (2) the resulting levels in human contact media ($\mu g/m^2$ of floor dust and $\mu g/m^3$ in air) derived from both outdoor and indoor sources. This model can be linked directly to the multimedia model to evaluate indoor/outdoor relationships. This model was used to evaluate the relative importance of various kinds of human factors in mediating human contacts with substances in air and dust. The loading of soil/dust on floor surfaces and the resuspension of particles from floors, for example, should increase as the number of household occupants increases. Increased loading of soil/dust on floors should in turn lead to more cleaning/vacuuming that redistributes pollutants onto contact surfaces throughout a house. For example, the tracking-in process, vacuuming, and particle penetration of a building shell tend to produce smaller sized particles in the indoor environment, making them more bioavailable.

B.6.3 CalTOX (California Total Exposure Model for Hazardous Waste Sites)

The Department of Toxic Substances Control (DTSC) within the California Environmental Protection Agency, has the responsibility for managing the State's hazardous-waste program. As part of this program, the DTSC funded the development of the CalTOX program. CalTOX has been developed as a set of spreadsheet models and spreadsheet data sets to assist assessing human exposures and defining soil clean-up levels at uncontrolled hazardous wastes sites (McKone 1993a, b, c). More recently, CalTOX has been modified for use in establishing waste classification for landfills and hazardous waste facilities in California. CalTOX addresses contaminated soils and the contamination of adjacent air, surface water, sediments, and ground water. The modeling components of CalTOX include a multimedia transport and transformation model, exposure scenario models, and add-ins to quantify uncertainty and variability. The multimedia transport and transformation model is a dynamic model that can be used to assess time-varying concentrations of pollutants introduced initially to soil layers or for pollutants released continuously to air, soil, or water. This model assists the user in examining how chemical and landscape properties impact both the ultimate route and quantity of human contact. Multimedia, multiple pathway exposure models are used in CalTOX to estimate average daily doses within a human population. The exposure models encompass twenty-three exposure pathways. The exposure assessment process consists of relating pollutant concentrations in the multimedia model compartments to pollutant concentrations in the media with which a human population has contact (personal air, tap water, foods, household dusts soils).

B.6.4 MMSOILS: Multimedia Contaminant Fate, Transport, and Exposure Model

MMSOILS was developed by EPA's ORD to estimate the human exposure and health risk associated with releases of contamination from hazardous waste sites (U.S. EPA 1992d). It is a multimedia model addressing the transport of a chemical in ground water, surface water, soil erosion, the atmosphere, and accumulation in food. The human exposure pathways considered in the methodology include: soil ingestion, air inhalation of volatiles and particulates, dermal contact, ingestion of drinking water, consumption of fish, consumption of plants grown on contaminated soil, and consumption of animals grazing on contaminated pasture. For multimedia exposures, the methodology provides estimates of human exposure through individual pathways and combined exposure through all pathways considered. The risk associated with the total exposure dose is calculated based on chemical-specific toxicity data. The intended use of MMSOILS is for screening and relative comparison of different waste sites, remediation activities, and hazard evaluation. The methodology can be used to provide an estimate of health risks for a specific site, but the uncertainty of the estimated risk may be quite large (depending on the site characteristics and available data) and this uncertainty must be considered in any decision-making process.

B.6.5 RESRAD (RESidual RADiation)

The Residential Radiation (RESRAD) model was developed by Argonne National

Laboratory to evaluate residual concentrations of radio nuclides in soil, concentrations of airborne radon decay products, external gamma radiation levels, surface contamination levels, and radio nuclide concentrations in air and water and to determine radiation dose and excess lifetime cancer risks to an on-site resident (a maximally exposed individual or a member of a critical population group).

RESRAD was developed for the U.S. DOE and is accepted for use in remedial action activities. RESRAD determines site-specific residual radioactive material cleanup guidelines based on calculations of the radiation dose to hypothetical residents or workers on the site. The nine environmental pathways considered in RESRAD are direct exposure, dust inhalation, radon, and ingestion of plant foods, meat, milk, aquatic foods, water, and soil.

RESRAD code has been adapted to include both chemical and radiological health risks. Other recent RESRAD developments include the incorporation of uncertainty analysis and decontamination and decommissioning analysis capabilities. The development of the code is funded by the DOE.

B.6.6 USES (Unified System for the Evaluation of Substances)

The Uniform System for the Evaluation of Substances (USES) (RIVM 1994), was developed in the Netherlands by the National Institute of Public Health and the Environment (RIVM); Ministry of Housing, Spatial Planning and Environment (VROM); and the Ministry of Welfare, Health, and Cultural Affairs (WVC). USES provides a single framework for comparing the potential risks of difference chemical substances released to multiple media of the environment. It is an integrated modeling system that includes multiple environmental media and multiple human exposure pathways. The exposure assessment in USES starts with an estimate of substance emissions to water, soil, and air during the various life-cycle stages of a substance and follows its subsequent distribution in the total environment. The result of this type of multi-media assessment are the Predicted Environmental Concentrations (PECs) and an estimate of the daily intake by human receptors. In general, PECs are compared to "no-effects" levels for organisms in the environment, which are derived by extrapolating single-species toxicity tests to field situations. The estimated daily intake by humans is compared to the "no-observed-adverse-effect" level for mammals or to the “no-effect” level for humans.

B.6.7 BEADS (The Benzene Exposure and Absorbed Dose Simulation)

BEADS (MacIntosh et al. 1995) was developed at the Harvard School of Public Health through support from EPA’s ORD. It is a population-based, multiple exposure pathway microenvironmental model of 24-hour average inhalation exposures and total absorbed doses of benzene. The model was developed: (1) to provide a tool for estimating the distribution of benzene personal air concentrations and total absorbed doses for a large population, (2) to examine the determinants of inter-individual variability of exposures and absorbed doses of benzene, and (3) to explore the accuracy and precision of predictions of population exposures and absorbed doses of benzene made with monitoring results from past field studies. A two-dimensional Monte Carlo simulation approach is used in the model to estimate the uncertainty about the predicted population exposure and absorbed dose distributions. A principal advantage of this approach to uncertainty analysis is that the relative contribution of the input variables to prediction uncertainty can be easily identified. Decisions can then be made regarding the appropriate measures to be taken to reduce the parameter uncertainty, where the overall goal is to minimize prediction uncertainty.

The BEADS model includes a probabilistic non-sequential (non-temporal) simulation of time activity patterns (TAP) and an anthropometric module used to correlate exposure factors in order to estimate absorbed dose (from inhalation, ingestion, and dermal absorption). Short term, high concentration exposures are not accounted for. The multimedia exposure and absorbed dose model underwent preliminary evaluation to estimate the benzene distribution of personal air concentration that would be expected for a large population depending on a microenvironment and exposure scenario in air (all via inhalation) or water (via ingestion, dermal uptake, or inhalation). Estimated distributions of personal and microenvironmental benzene exposures compared well with previous monitoring results (TEAM–Total Exposure Assessment Methodology) except at the upper ends.

B.6.8 DERM (Dermal Exposure Reduction Model)

The physical-stochastic model DERM, was developed by Stanford's Environmental Engineering and Science Group to estimate personal dermal exposure incurred via multiple contact mechanisms as a function of time (Zartarian 1996). This is the first exposure model to calculate dermal exposure as a function of actual human activity data. An important output of DERM is the dermal exposure profile, which plots mass of pollutant loading on the skin as a function of time. Such profiles are the basis of understanding the pathways by which dermal and non-dietary ingestion exposure are incurred (*e.g.*, liquid immersion, surface contact with liquids, soil, or dust, aerosol deposition, hand-to-mouth contact). DERM is a personal, physical-stochastic model designed to evaluate the sources of uncertainty in the calculations, to understand the important dermal exposure contact pathways, and to help determine the best ways to control those factors that contribute most significantly to exposure. DERM has also been designed to assess ingestion exposures for hand-to-mouth activities.

B.6.9 SCREAM2 (South Coast Risk and Exposure Assessment Model, ver. 2)

The SCREAM2 (Rosenbaum et al. 1994) was developed with support from California's South Coast Air Quality Management District and provides the ability to model both inhalation and multipathway non-inhalation exposures. A submodel, called MULTPATH, calculates population exposures to air toxics through non-inhalation pathways. The MULTPATH submodel includes the following pathways: soil ingestion, soil dermal contact, home-grown produce ingestion, commercial (locally-grown) produce ingestion, commercial (locally-raised) animal product ingestion, surface drinking water (local source) ingestion, fish (local source) ingestion, and breast milk ingestion. Average daily doses of a pollutant to the population are estimated from concentrations in each medium on the basis of age-specific ingestion rates and body weights and local population age profiles. Exposure estimates are made with respect to contamination of commercial foodstuffs (produce and animal products) and surface water used for drinking and/or fishing by assuming that they are consumed entirely and uniformly by the population of the modeled area in proportion to the average ingestion rates for each age group. The individual carcinogenic health risk associated with ingestion exposure over a 70-year lifetime is estimated as the product of the dose and a cancer potency slope. MULTPATH requires site-specific information on the locations and yields of all commercial produce and commercial animal-raising operations. In addition, the locations and information on certain physical parameters of all water bodies used as sources of drinking water or fishing are required.

For inhalation exposures, the 24-hourly concentrations for each census block group are estimated using a Gaussian air dispersion– and mapping modules. For each source, the model calculates ground-level concentrations as a function of radial distance and direction from the source for a set of receptors laid out in a radial grid pattern. The concentrations represent the steady-state concentrations that would occur with constant emissions and meteorological parameters.

The inhalation exposure module accounts for mobility patterns of the population, indoor-outdoor exposure concentration differences, and physical exercise levels. The module estimates exposures for each individual census block group, aggregating exposure throughout the modeled area for a number of subregions, called exposure districts. Exposure is estimated for 12 basic population age/occupation groups which are further subdivided into 56 subgroups, distinguished by their hourly activity patterns. For each hour, a subgroup is assigned to a geographic location (*i.e.*, either a home or work district), one of several different indoor or outdoor microenvironments, and one of three physical exercise levels (low, moderate, or heavy). There are population activity patterns defined for weekdays, Saturdays, and Sundays.

In order to track the geographic locations of the population from hour to hour, the inhalation exposure/risk module again divides the 56 subgroups into cohorts, defined on the basis of common age-occupation groupings, and again by home and work exposure districts. The population composition and mobility data are compiled at the exposure-district level, while concentrations are for the smaller census block-group level.

SCREAM2 can use the Indoor Air Quality Model (IAQM) submodel to calculate indoor pollutant concentrations. IAQM simulates indoor air quality by means of a dynamic mass balance equation, with a building being represented by a single compartment. Outdoor air is permitted to leak into and out of the building, and indoor recirculation and makeup air can be supplied as appropriate through simulation of a heating, ventilation, and air conditioning (HVAC) system. In addition, indoor sources, which are specified in terms of source strength and time profile, can be modeled with the IAQM. Pollutant losses indoors are simulated in terms of adsorption onto surfaces or deposition due to settling, with surface reactivity or deposition rates dependent on the pollutant.

B.6.10 Integrated Spatial Multimedia Compartmental Model (ISMCM)

The Integrated Spatial Multimedia Compartmental Model has been under development with the School of Engineering and Applied Science at the University of California Los Angeles for approximately the last 15 years. A newer version of the ISMCM, called MEND–TOX, is currently undergoing evaluation at the EPA ORD's National Exposure Research Laboratory (NERL).

The ISMCM considers all media in one integrated system. It includes both spatial and compartmental modules to account for complex transport of pollutants through the ecosystem. Assuming mass conservation, ISMCM is able to predict transport based on a mechanistic description of environmental processes, including estimation of intermedia transfer factors.

The ISMCM is not structured to incorporate uncertainty/variability analyses directly into the model operation. Furthermore, the links and compartments (spatial configuration) of the ISMCM are predetermined, thereby making it less useful in a system that is to be fully integrated.

B.6.11 Indirect Exposure Methodology (IEM) Model

The U.S. EPA began developing the Indirect Exposure Methodology (IEM) in the 1980s. The IEM consists of fate and transport algorithms that estimate the media concentrations resulting from the multipathway transfer of air pollutants to soil, vegetation, and water bodies. The algorithms in IEM are designed to predict exposures for pollutants for which indirect impacts may be important (*i.e.*, organic and inorganic pollutants that tend to be long-lived, bioaccumulating, non- [or at most semi-] volatile, and more associated with soil and sediment than with water). An interim document summarizing the IEM methodology was published in 1990 (U.S. EPA 1990b), and a major addendum was issued in 1993 (U.S. EPA 1993b). The Agency's Office of Solid Waste and Emergency Response (OSWER) has adapted IEM and compiled detailed information on many of IEM's input parameters and algorithms in the *Human Health Risk Assessment Protocol for Hazardous Waste Combustion Facilities* (U.S. EPA 1998e). The algorithms in IEM are under continuous refinement, and revised documentation addressing SAB and public comments on the 1993 Addendum is pending (U.S. EPA 1999h). This revised document no longer uses the IEM terminology; instead, the document refers to MPE (multiple pathways of exposure) assessment.

The IEM estimates human exposure to pollutants via several routes, including inhalation, dermal contact, and food, water, and soil ingestion. Exposures are estimated using environmental media concentrations, transfer factors (*e.g.*, bioaccumulation factors) where appropriate, and measures of human activity and exposure characteristics (*e.g.*, consumption rates for food types) such as those available in EPA's *Exposure Factors Handbook* (U.S. EPA 1997b). The IEM is designed to estimate intakes for specific, predetermined receptor scenarios (*e.g.*, subsistence gardener, recreational fisher, average urban resident) that may be indicative of high-end or average exposures to a pollutant.

Because it is designed to estimate exposure for individuals classified into specific scenarios, IEM does not readily allow for the modeling of a distribution of exposures within a population. It is not designed to provide estimates of population exposures. In addition, IEM is set up to model a long-term emission source, and the fate and transport component of IEM consists of a set of linked, one-way algorithms that do not allow for tracking transformations between different chemical species or feedback between different media. Pollutants are input to the model as annual average air concentrations and wet and dry deposition rates for a specific location or as areal averages for a given space (*e.g.*, a watershed). Thus, the model cannot provide a detailed time series estimation of media concentrations and the resulting human exposures, and spatial variations in exposure can be approximated only through substantial site-specific model adjustment and repeated model runs. In addition, IEM is a deterministic model and is not designed to estimate the uncertainty or variability associated with exposure estimates. These characteristics make IEM suitable for scenario-specific, screening-level exposure assessments and the determination of exposure routes of potential concern for a long-term emission source but less appropriate for estimating distributions of population exposures over time and space and across various pathways.

B.7 EXPOSURE SIMULATION MODEL SYSTEMS

In addition to exposure models, there are a number of exposure modeling systems. These are systems or libraries that can contain transport models, exposure models, data files, and the associated software for linking these models with the various input and output files.

B.7.1 GEMS (Graphical Exposure Modeling System)

The EPA's OPPT developed the Graphical Exposure Modeling System (GEMS) to support exposure and risk assessments by providing access to single medium and multimedia fate and exposure models, physical and chemical properties estimation techniques, statistical analysis, and graphics and mapping programs with related data on environments, sources, receptors, and populations. Under development since 1981, GEMS provides analysts with an interactive, easily learned interface to various models, programs, and data needed for exposure and risk assessments. PC-GEMS (GSC 1988) is a stand-alone version of GEMS that can be run on a personal computer.

The environmental models in GEMS are atmospheric, surface water, land unsaturated (soil) and saturated (ground water) zones, and multimedia in nature. Methods for estimating octanol-water partition and adsorption coefficients, bioconcentration factor, water solubility, melting and boiling point, vapor pressure, Henry's constant, acid dissociation constant, lake/stream volatilization rate, and atmospheric half-life are available. Data sets are related to environmental characteristics (climate, soil, rivers, ground water, vegetation), source releases (POTWs and industrial water discharges, Census business patterns, RCRA permit sites), and receptors (population and household estimates for 1970, '80, '90, and '95 by small area census district; and drinking water facility information).

B.7.2 THERdbASE (Total Human Exposure Risk database and Advanced Simulation Environment)

THERdbASE has been developed by EPA's ORD as a PC-based computer modeling and database system that contains exposure and risk related information. The system provides a framework for the construction of a suite of exposure and risk related models within the Modeling Engine by using information available in data files within the Database Engine. Data can be viewed as a table, coded fields can be viewed as decoded fields, fields can be set to "show" or "hide" mode, and multiple data files can be viewed at the same time. In the "advanced" mode, user files can be edited. Data records can be queried and simple statistics (summary statistics — mean; standard deviation; minimum and maximum; percentile values at desired intervals; and linear regression on two numerical data fields) can be performed. Data can be printed, saved, or exported. New user files can be created and data can be imported. Input to models is achieved through a standardized procedure. Inputs can be provided as single values, custom distributions (normal, lognormal), distributions based on data files present in THERdbASE, or as specific percentile values. Efficient algorithms are provided to optimally access input data, to perform the numerical simulations, and to generate appropriate output data. Multiple model runs can be done through a batch process. Results can be output as either THERdbASE data files or as pre-set graphs (U.S. EPA 1998g).

Information about THERdbASE is available on the EPA's Internet website (http://www.epa.gov/nerlpage/heasd/therdbase.htm). The Internet version of THERdbASE includes the following models:

- Location Patterns
- Chemical Source Release - Instantaneous Emission
- Chemical Source Release - Timed Application
- Indoor Air (2-Zone)
- Indoor Air (N-Zone)
- Exposure Patterns For Chemical Agents
- Benzene Exposure Assessment Model (Beam)
- Source Based Exposure Scenario (Inhalation + Dermal)
- Film Thickness Based Dermal Dose
- PBPK Based Dermal Dose

The Internet version of THERdbASE also includes the following databases:

- 1990 Bureau of Census Population Information
- California Adult Activity Pattern Study (1987 - 88)
- AT&T-sponsored National Activity Pattern Study (1985)
- 1992-94 National Human Activity Patterns Study (NHAPS)
- Chemical Agents from Sources
- Chemical Agent Properties
- Air Exchange Rates
- Information from EPA's TEAM (Total Exposure Assessment Methodology) Studies
- Information from EPA's NOPES (Non-Occupational Pesticides Exposure Study) Studies

• Human Physiological Parameters

B.7.3 MEPAS (Multimedia Environmental Pollutant Assessment System)

The Multimedia Environmental Pollutant Assessment System (MEPAS) (Strenge and Chamberlain 1995, Droppo et al. 1992) was developed by Battelle Pacific Northwest Laboratory (PNL) for the U.S. Department of Energy. The system was developed to rank DOE sites having potential hazardous chemical and radioactive releases. The key objective of MEPAS is to rank sites by calculating human health risk to the population surrounding the site. MEPAS calculates "hazard potential index" (HPI) values for a site by summing up risk factors associated with various exposure scenarios. This system has wide applicability to a range of environmental problems using air, ground water, surface water, overland, and exposure models. MEPAS integrates source, transport, and exposure models into a single system. The algorithms in MEPAS accommodate the following ten components: 1) source terrain, 2) overland pathway, 3) ground water (vadose and saturated zones) pathway, 4) surface water pathway, 5) atmospheric pathway, 6) exposure routes, 7) hazard assessment (chemical carcinogens / non-carcinogens; radio nuclides), 8) pollutant/transport and exposure scenarios, 9) a user-friendly PC shell, and 10) a chemical database.

Pollutant transport media are ground water, overland flow, surface water, and atmosphere. Human uptake occurs through ingestion (of contaminated water, soil, crops, animal products, and aquatic foods), inhalation (of airborne pollutants), and dermal contact (with chemicals and radio nuclides). The hydrologic media consists of the hydrologic source term, unsaturated and saturated ground water zones, and surface water/runoff. The source term can be computed internally or specified at receptor locations or by specified flow. The source term geometries include point, line, and area sources. Limitations of the hydrologic pathway include negligible leaching of the source by ground water, and flow in the virtual direction only.

The atmospheric pathway consists of the atmospheric source term and atmospheric transport processor. Source terms consist of point sources and area sources. Atmospheric transport of pollutants utilizes an enhanced Gaussian plume model, and computes long term exposure for a sixteen sector grid using average stack parameters. Enhancements to the plume model include deflection of wind speed to account for variability in local surface roughness, and can consider radioactive decay depletion and first order chemical reactions. Only simple sources can be modeled, and particulate pollutants originate from area sources only.

MEPAS calculates an average dose over 70 years time increments for a number of user specified receptor locations. Dose is calculated for each transported pollutant. For radioactive pollutants the dose is expressed as the effective dose equivalent from each pollutant. MEPAS uses the ICRP dose conversion factors to convert the rate of exposure to dose.

B.7.4 EML/IMES (Exposure Models Library / Integrated Model Evaluation System)

The Exposure Models Library (EML) was developed by the U.S. EPA's ORD and is a collection of exposure models distributed in a CD-ROM (U.S. EPA 1996c). The purpose of this disk is to provide a compact and efficient means to distribute exposure models, documentation, and the Integrated Model Evaluation System (IMES). The EML disk contains over 120 models which may be used for exposure assessments and transport modeling. The model files may contain source and/or executable code, sample input files, and other data files, sample output files, and in many cases, model documentation in WordPerfect®, ASCII text, or other similar formats. IMES assists in selecting appropriate models, provides literature citations on model validations, and demonstrates model uncertainty protocols. The IMES software is an MS-DOS application, can be used on an Intel-based PC, and is capable of running on a network. Model codes and documentation can be downloaded from the CD-ROM to a hard drive. The most recent version, which is the third edition, has an HTML interface to view model directories and Internet source for some models.

B.7.5 MENTOR (Modeling ENvironment for TOtal Risk)

The Modeling ENvironment for TOtal Risk (MENTOR) project, is being developed through funding from EPA's National Exposure Research Laboratory (NERL). The objective of the on-going MENTOR project is to develop, apply through case studies, and evaluate state-of-the-art computational tools, that will support multipathway, multiscale source-to-dose studies and exposure assessments for a wide range of environmental pollutants. Particular emphasis in MENTOR is placed on integrating methods for prognostic and diagnostic exposure/dose analyses, by utilizing, in combination, environmental, microenvironmental, and biomonitoring information to evaluate assumptions regarding routes and pathways of exposure.

MENTOR merges the methods and tools of the comprehensive Exposure and Dose Modeling and Analysis System (EDMAS) with those currently available in pNEM, and extends them for application to situations that are relevant to multimedia and multipathway exposures. EDMAS is an expandable library of interlinked computation modules (Georgopoulos et al. 1997). MENTOR incorporates models, databases, and analytic tools which can probabilistically estimate exposures (and doses) to individuals, populations, and susceptible subpopulations as well as predict and diagnose the complex relationships between source and dose. MENTOR is designed as a multiscale modeling system, that allows following in a mechanistically consistent manner the evolution of physicochemical phenomena over spatial scales ranging from geographic regions to personal and residential microenvironments. It provides a consistent link with biological uptake and disposition models. MENTOR is also multiscale in time, designed to support modeling of processes in ranges from minutes to decades.

MENTOR has a modular structure with an interface that offers linkage to both a Geographic Information System (ArcView and ArcInfo) and a relational database management system (Oracle) for "defining" an application or case study. MENTOR incorporates libraries of environmental and biological process models, including macroenvironmental, ecological/food-web, local multimedia, microenvironmental, activity pattern/exposure event, biological fate and transport, and dose response modules. MENTOR will eventually provide an extensible set of ready-to-use methodological tools, as well as linkages to relevant databases, for performing assessments of exposure/dose for populations or specific individuals, and for a variety of user-defined scenarios.

The MENTOR development and application effort is being pursued at the Computational Chemodynamics Laboratory (CCL) of the Environmental and Occupational Health Sciences Institute (EOHSI), which is a joint project of the University of Medicine and Dentistry of New Jersey (UMDNJ) and Rutgers University.

B.7.6 MODELS-3/Multimedia Integrated Modeling System (MIMS)

The U.S. EPA ORD's NERL is developing Models-3 Community Multi-scale Air Quality (CMAQ) modeling system. It is a flexible software system designed to simplify the development and use of environmental assessment and decision support tools for a wide range of applications from regulatory and policy analysis to understanding the interactions of atmospheric chemistry and physics. This newest generation of environmental modeling software has been under development for the past seven years.

Models-3, in combination with CMAQ, form a third generation air quality modeling and assessment system. First generation air quality models dealt with tropospheric air quality with simple chemistry at local scales using Gaussian plume formulation as the basis for prediction. Second generation models covered a broader range of scales (*i.e.*, local, urban, and regional) and pollutants, addressing each scale with a separate model and often focusing on a single pollutant. Third generation models treat multiple pollutants simultaneously up to continental scales and incorporate feedback between chemical and meteorological components. Future development is planned for a fourth generation system which would extend linkages and process feedback to include air, water, land, and biota to provide a more holistic approach to simulation of transport and fate of chemical and nutrients throughout an ecosystem (U.S. EPA 1998f). This system, called the Multimedia Integrated Modeling System (MIMS), is described below.

Models-3 has a unique framework and science design that enables scientists and regulators to build their own modeling systems to suit their needs. The CMAQ system has capabilities for urban to regional-scale air quality simulation of tropospheric ozone, acid deposition, visibility, and fine particles. The Models-3 framework contains components that assist the model developer with creating, testing, and performing comparative analysis of new versions of air quality models and enables the user to execute air quality simulation models and visualize the results. The overall goal of Models-3 is to simplify and integrate the development and use of complex environmental models, beginning with air quality and deposition models (U.S. EPA 1998f).

MIMS will have capabilities to represent the transport and fate of nutrients and chemical stressors over multiple scales. It will be designed to improve the environmental management community's ability to evaluate the impact of air and water quality and watershed management practices on stream and estuarine conditions. The system will provide a computer-based problem solving environment for testing understanding of multimedia (atmosphere, land, water) environmental problems, such as the movement of chemicals through the hydrologic cycle, or the response of aquatic ecological systems to land-use change, with initial emphasis on the fish health endpoint. The design will attempt to combine the state-of-the-art in computer science, system design, and numerical analysis (*i.e.* object oriented analysis and design, parallel processing, advanced numerical libraries including analytic elements) with the latest advancements in process level science (process chemistry, hydrology, atmospheric and ecological science). The problem solving environment will embrace the watershed/airshed approach to environmental management, and build upon the latest technologies for environmental monitoring and geographic representation.

B.7.7 SHEDS (Stochastic Human Exposure and Dose Simulation) Model

The Stochastic Human Exposure and Dose Simulation (SHEDS) Model is a probabilistic, physically-based model that simulates aggregate exposure and dose for population cohorts and multimedia pollutants of interest. It is being developed by the U.S. EPA ORD's NERL. At present the model is applied to assess children's exposures to pesticides (SHEDS-Pesticides) and population exposures to PM (SHEDS-PM). The key objectives of SHEDS are: (1) to improve the risk assessment process by predicting both inter-individual variability and uncertainties associated with the upper percentiles (*e.g.*, >90th percentile) of population exposure and dose distributions; (2) to improve the risk management process by identifying critical exposure routes and pathways; and (3) to provide a framework for identifying and prioritizing measurement needs and to formulate the most appropriate hypotheses and designs for exposure studies.

SHEDS-PM estimates the population distribution of PM exposure by sampling from distributions of ambient PM concentrations and from distributions of emission strengths for indoor sources of PM, such as cigarette smoking and cooking. A steady-state mass balance equation is used to calculate PM concentrations for the home microenvironment. The physical factors data used in the equation (*e.g.*, air exchange rate, penetration rate, deposition rate) are also sampled from distributions. Non-residential microenvironmental concentrations are calculated based on penetration of outdoor PM and indoor sources. Additional model inputs include demographic data for the population being modeled and human activity pattern data from the National Human Activity Pattern Survey (NHAPS). Output from the SHEDS-PM model includes distributions of PM exposures in various microenvironments (*e.g.*, indoors at home, in vehicles, outdoors) and the relative contributions of these various microenvironments to the total exposure.

The first generation of SHEDS-PM has been applied to the population of Vancouver, Canada using spatially interpolated ambient PM10 measurements (Özkaynak et al. 1999a, b) Subsequent generations will focus on modeling both PM10 and PM2.5 exposure and dose in a selected U.S. city.

SHEDS-Pesticides predicts children's aggregate population exposure and dose to pesticides. It simulates individuals from the user-specified population cohort by selecting daily sequential time/location/activity diaries from surveys contained in EPA's CHAD (*e.g.*, the National Human Activity Pattern Survey). For each individual, SHEDS-Pesticides constructs daily exposure and dose time profiles for the inhalation, dietary and non-dietary ingestion, and dermal contact exposure routes, then aggregates the dose profiles across routes. A single-compartment pharmacokinetic component has been incorporated into the first generation SHEDS-Pesticides model to predict real-time pollutant or metabolite concentrations in the blood compartment or eliminated urine. Exposure and dose metrics of interest (*e.g.*, peak, time-averaged, time-integrated) are extracted from the individual's profiles, and the process is repeated thousands of times to obtain population distributions. This approach allows identification of the relative importance of routes, pathways, and model inputs. Two-stage Monte-Carlo sampling is applied to predict the range and distribution of aggregate doses within the specified population and the uncertainties associated with percentiles of interest.

SHEDS-Pesticides samples, for each individual, location-specific air, dust, soil, and surface residue levels; meal-specific food and beverage residues; exposure factors (*e.g.*, residue-to-skin transfer efficiency, saliva and washing removal efficiency, soil adherence, surface area contacted); uptake factors (*e.g.*, inhalation and dietary absorption fractions); and pharmacokinetic rate constants (*e.g.*, dermal absorption, gastrointestinal absorption, elimination) from user-specified probability distributions. For each location/activity combination in the individual's diary, SHEDS-Pesticides combines the air concentration, activity-specific inhalation rate (derived from distributions of MET energy expenditures), and inhalation absorption fraction to estimate real-time inhalation absorbed dose. For each eating or drinking event, SHEDS-Pesticides combines the mass residue ingested by the ingestion absorption fraction to obtain mass in the gastrointestinal tract, then applies a gastrointestinal absorption rate constant to estimate real-time mass in the blood compartment. If the eating event is non-dietary, the mass of residue ingested is that on the object mouthed or the skin at that instant in time. The dermal loading over time is obtained by simulating exposures from discrete dermal contact events (*i.e.*, contacts between the skin surface and different objects such as smooth surfaces, textured surfaces, mouth, turf) within each macro-activity. Probabilities of skin contacts with different surfaces for a given contact event are obtained from the contact frequency and duration information collected via videography studies. For each dermal contact event, the model combines available mass on the skin by a dermal absorption rate constant to estimate real-time dermal absorbed dose.

To help meet the requirements of the Food quality Protection Act of 1996 (FQPA), the initial focus of the SHEDS-Pesticides model has been residential exposures of children to pesticides. Model estimates for chlorpyrifos have been obtained for several application methods (*i.e.*, broadcast, crack, and crevice) and age groups (0-4 years, 5-9 years) for acute, short-term, and chronic post-application time periods, and then weighted with available pesticide use and frequency information to develop aggregate population estimates. A paper describing the initial SHEDS-Pesticides modeling framework, presenting the chlorpyrifos case study, and demonstrating that the modeled estimates compare well against available published measurement data has been submitted for publication (Zartarian et al. 1999).

While the first generation SHEDS-Pesticides model was developed with a special emphasis on characterizing critical exposure pathways and factors for residential exposures of children to pesticides, the next generation will characterize both aggregate and cumulative dose associated with human exposure (*i.e.*, for both adults and children) to a variety of environmental pollutants in addition to pesticides, including other persistent organic pollutants, metals, and air toxics. SHEDS-Pesticides will eventually be expanded to include source-to-concentration (*i.e.*, fate and transport models) and more complete exposure-to-dose models (pharmacokinetic or dosimetric models).

Each iteration of SHEDS will use the best available data to identify critical pathways of human exposure and dose and the major uncertainties in those pathways. Model inputs and assumptions will continue to be reined as new measurement data become available (*e.g.*, pesticide usage survey data, residue and concentration distributions in space and time, residue-to-skin transfer efficiencies, uptake data, microlevel activity data, emission source strengths, air exchange rates, penetration rates). The model will be tested against field measurement programs for refinement and subsequent evaluation.

Table B-1
Model Features and the Exposure Models Associated with Each Feature

Feature	Model	Remarks
Short-term (≤ 1 h) exposure events	CPIEM	Other built-in time scales include: 24 hours, 12 hours (daytime), 12 hours (nighttime), and 8 hours.
	pNEM	Inhalation exposures can be calculated for i minute to 24 hours depending on the pollutant. Exposures are generally for 1-hour (5-minute duration for SO_2). However, activities can be as short as 1-minute in duration.
	HAPEM-PS	Annually averaged 1-hour increments.
	HAPEM	Seasonally (3-month) averaged 1-hour increments.
	AirPEx	15-minutes
	SHAPE	Exposures are generally for 1-hour. However, activities can be as short as 1-minute in duration.
	DERM	Dermal exposures are estimated over the day based on dermal contact events ranging from seconds to minutes.
	SHEDS (under development)	Inhalation exposures can be calculated for 1 minute to 12 hours, depending on the pollutant and diary selected. Dermal and non-dietary ingestion exposures can be as short as a 5-second duration. Diaries are used to determine ingestion events. Modeled dietary ingestion exposures for each eating and drinking event are assumed instantaneous, but absorption is calculated on a 30-minute time scale.
	BEAM	1 hour.
	pHAP	1 hour.
Long-term exposure events	CalTOX	Annual.
	SHEDS (under development)	Daily exposure and dose profiles could be repeated over longer durations based on multi-day activity and contact frequency information.
	HEM	Annual.
	SCREAM2	Annual.
Exposure media	CPIEM	Indoor air (multiple microenvironments).
	pNEM	Indoor air and outdoor air.
	HAPEM	Indoor air and outdoor air.
	AirPEx	Indoor air and outdoor air.

Feature	Model	Remarks
	HEM	Indoor air and outdoor air.
	SHAPE	Indoor air and outdoor air.
	BEAM	Indoor air and outdoor air.
	pHAP	Indoor air and outdoor air.
	CONSEXPO	Indoor air, personal air, and contact with surfaces (both oral and dermal).
	CalTOX	Indoor air; outdoor air; soil; house dust; tap water; food from home gardens and locally-produced fruits, vegetables, grains, fish, meat, milk, eggs; and dairy products.
	SHEDS (under development)	Indoor air; outdoor air; soil; house dust; surface residues (indoor and lawn); hand and object residues; tap water; food and beverage residues
	MMSOILS	Indoor air; outdoor air; soil; house dust; tap water; food from home gardens and locally-produced fruits, vegetables, grains, fish, meat, milk, eggs; and dairy products.
	USES	Indoor air; outdoor air; soil; house dust; tap water; food from home gardens and locally-produced fruits, vegetables, grains, fish, meat, milk, eggs; and dairy products.
	BEADS	Indoor air, outdoor air, and tap water.
	SCREAM2	Indoor air; outdoor air; soil; tap water; food from home gardens; locally-grown produce; locally-raised animal products, including fish; and breast milk.
	DERM	Liquid, air, soil on surfaces, dust on surfaces, residues on surfaces.
	DERMAL	Contact with surfaces (dermal).
Models inhalation only	CPIEM	Designed for indoor exposures to numerous pollutants.
	pNEM	Models are pollutant-specific (*e.g.*, ozone, carbon monoxide, sulfur dioxide). Current development is on CO-version.
	HAPEM	For criteria and modeled air toxic pollutants.
	AirPEx	Default values available for benzene, B(a)P, ozone, and PM.
	HEM	Multiple gas- and particle-phase agents from outdoor sources.
	SHAPE	Model designed for inhalation exposures to CO.
	BEAM	Model for benzene only.
	pHAP	Multiple gas- and particle-phase agents from outdoor sources. Has been tested using benzene.
Models non-inhalation routes of exposure	CONSEXPO	Inhalation, ingestion, and dermal contact of chemicals from consumer products. Indoor sources only.
	CalTOX	Inhalation, ingestion, and dermal contact of organic chemicals and some metals.

Feature	Model	Remarks
	MMSOILS	Inhalation, ingestion, and dermal contact of organic chemicals and metal species from hazardous waste sites.
	USES	Inhalation, ingestion, and dermal contact of organic chemicals and some metal species.
	BEADS	Inhalation, ingestion, and dermal contact to benzene only.
	SHEDS (under development)	Inhalation, dietary and non-dietary ingestion, dermal contact for multimedia pollutants.
	SCREAM2	Inhalation, ingestion, and dermal contact to numerous modeled air toxics.
	DERM	Dermal exposure to pesticides.
	DERMAL	Calculates screening-level estimates of annual individual dermal potential dose rates to components of 16 consumer product categories.
Explicit treatment of variability	CPIEM	Several parameters are sampled from distributions, including the concentration data. A variety of formats for describing the concentration distribution is allowed by the model, including provision of a data file containing the concentration values. A random number seed can be selected by the user or the model can use the system's clock to determine the seed.
	CalTOX	Variability in exposure factors and in landscape factors are explicitly represented by probability distributions.
	pNEM	Environmental, demographic (*e.g.*, activity pattern and ventilation data), and mass balance inputs are characterized by distributions.
	HAPEM	Most input parameters are characterized by distributions.
	AirPEx	Exposure distributions for the population are characterized by the normalized cumulative frequency distribution.
	SHEDS (under development)	Model samples from user-specified input probability distributions for residues and exposure factors. Monte Carlo sampling allows analyses of input and output variability.
	HEM	
	SHAPE	Model generates a hypothetical population, sampling each descriptive parameter of an individual (*e.g.*, age, gender, body mass) from a user-specified distribution function.
	DERM	Variability quantified by applying bootstrap method to dermal exposure estimates for individuals
	BEAM	
	pHAP	
Explicit treatment of uncertainty	CPIEM	User specifies all inputs. Then, the model is run several times with all inputs kept constant except the random number seed. Variability for each output parameter across repeated model runs is characterized through a measure such as the coefficient of variation.
	SHEDS (under development)	Two-stage Monte Carlo sampling allows for explicit characterization of both uncertainty and variability. Model samples from user-specified input probability distributions and their associated uncertainty distributions.

Feature	Model	Remarks
	CalTOX	All chemical-specific property data are represented by probability distributions.
	HEM	
	pNEM	The model is generally run 10 times using a Monte Carlo simulation approach for each regulatory scenario analyzed.
Mass balance approach for indoor concentrations	pNEM	Mass balance model accounts for outdoor concentration, air exchange rate, building volume, building penetration rate, deposition rate, and indoor emission rates and usage patterns for some indoor sources.
	SHEDS (under development)	Mass balance model accounts for outdoor concentration, air exchange rate, building volume, and indoor emission rates, and usage patterns
	CPIEM	Uses a mass balance equation, based on the principle of conservation of mass, to estimate concentration distributions for specific types of indoor environments such as residences, offices, and schools.
	SCREAM2	Optional use of mass balance model that accounts for outdoor concentration, air exchange rate, and indoor emission rate.
Regression or I/O ratios for indoor concentrations	HAPEM	Uses microenvironmental factors.
	AirPEx	Parameters relating concentration measured at monitoring site to four macroenvironments (rural, urban, city, and transit) which are in turn related to three indoor microenvironments (home, vehicle, elsewhere) by I/O ratios. Also, three additive terms account for indoor sources in the same three microenvironments.
	SHEDS (under development)	For certain microenvironments, empirical mass balance models in the form of regressions are used.
	HEM	Uses I/O ratios for microenvironments.
	SHAPE	Exposure concentrations are obtained by applying a superposition principle to contributions from the ambient and different microenvironments.
	BEAM	Same as SHAPE.
	SCREAM2	Optional use of I/O ratios for microenvironments.
Includes ventilation rate	pNEM	Ventilation rate (V_E) value estimated based on estimated body mass, gender, and other information from energy expenditure literature for each exposure event.
	SHEDS (under development)	Ventilation rate (V_E) value estimated based on estimated body mass, gender, and other information from energy expenditure literature for each exposure-event.
	CPIEM	Breathing rates supplied by the model are specific to three age/gender groups (adult males, adult females, and children under age 12) and four activity levels (resting, light, moderate, and heavy).
	SCREAM2	For each hour, the activity pattern of each subgroup is assigned to one of three activity levels (low, moderate, or heavy). The user may designate enhancement of inhaled dosage of the pollutant for the various activity levels with scaling factors.

Feature	Model	Remarks
	AirPEx	Ventilation rate is a function of a person's body mass and level of activity. Uses five levels of activity, ranging from "sleeping" to "heavy exercise."
Can estimate dose	pNEM	The CHAD database provided an activity indicator for each exposure event. Each activity type was assigned a distribution of values for the metabolic equivalent of work (MET). The MET is dimensionless, given by the ratio of the rate of energy expenditure during a particular activity (expressed in kcal/min) and a person's typical resting metabolic rate (also expressed in kcal/min).
	SHEDS (under development)	Inhalation: For each modeled individual's sequential location/activity combination in daily diaries, model combines air concentration, activity-specific inhalation rate (derived via METs), and absorption fraction to estimate inhalation absorbed dose. Next generation will include more PK models to calculate dose. Ingestion: For each eating and drinking event, model combines mass residue ingested and absorption fraction to obtain mass in gastrointestinal (GI) tract, then applies a GI absorption rate constant to estimate mass in blood compartment. Dermal: For each dermal contact event, model combines available mass on skin and dermal absorption rate constant to estimate dermal absorbed dose. To obtain aggregate absorbed and eliminated dose, model sums time profiles across all routes.
	CPIEM	Breathing rates and activity levels are used by the model to calculate the potential inhaled dose received by each individual in each microenvironment.
	SCREAM2	Average daily doses of a pollutant to the population are estimated from concentrations in each medium on the basis of age-specific ingestion rates and body weights and local population age profiles.
Includes indoor sources	CPIEM	The model samples values from user-specified distributions for emission rates for indoor sources.
	SHEDS (under development)	The model samples values from user-specified distributions for indoor source concentrations.
	pNEM	Includes CO emitted by gas stove operation and passive smoking.
	HAPEM	Includes an additive term for indoor source contributions (user specified).
	SCREAM2	Includes an additive term for indoor source contributions (user specified).
Includes smoking as a source	pNEM	Contribution from smoking is modeled.
	SHEDS (under development)	Contribution from smoking is modeled.

Feature	Model	Remarks
Calculates exposures of commuters	pNEM	The populations of the commuting cohorts (assumed to include all working cohorts) were determined by the expression: *Com(d,h,f,w) = Pop(d,h,f) x Com(h,w)/Work(h)* where *Com(d,h,f,w)* is the number of persons in the commuting cohort associated with demographic group *d*, home district *h*, cooking fuel *f*, and work district *w*; *Pop(d,h,f)* values provided an estimate of the population of each non-commuting cohort residing within home district *h*; *Com(h,w)* is the number of workers in all demographic groups that commute from home district *h* to work district *w*; and *Work(h)* is the total number of workers in home district *h*. Estimates of *Work(h)* were developed from census data specific to each district. The in-vehicle concentration is calculated using a mass balance model.
	SHEDS (under development)	Exposures of commuters are modeled. A similar approach to pNEM is being considered.
	HAPEM	Commuting patterns of workers between exposure districts are modeled. The “travel time to work” data from the 1990 census are used to develop the commuting patterns. A program uses these data to build an array of probabilities of the movement of working commuters for each census tract-to-tract combination.
	SCREAM2	Commuting patterns of workers between exposure districts are modeled. The patterns were estimated from travel survey data collected by the Southern California Association of Governments in a manner similar to pNEM/CO.
Includes dispersion algorithms to calculate outdoor air concentrations	SCREAM2	Uses a Gaussian model formulation and climatological data to estimate long-term average concentrations as a function of radial distance and direction from a source for a set of receptors laid out in a radial grid pattern.
	SHEDS (under development)	Uses Bayesian spatial and temporal interpolation methods to estimate outdoor air concentrations in different census tracts.
	HEM	Uses the Industrial Source Complex Long-Term (ISCLT2) Model for estimating dispersion.

Table B–2[3]
Strengths and Weaknesses of Different Models and Modeling Systems

Model	Strengths	Weaknesses
pNEM/CO (inhalation)	1. Most input parameters are probabilistic. 2. Can calculate delivered dose as a function of the pollutant concentration and ventilation rate values assigned to the event and the demographic characteristics of the cohort. 3. Mass balance model for indoor microenvironments. 4. Calculates the exposures to the portion of the population that commute to work. 5. Estimates exposures to those exposed to passive smoking.	1. Single exposure route (inhalation) only. 2. Each version of pNEM is specific to a single pollutant.
CalTOX (multimedia)	1. Multipathway and multimedia. 2. All input parameter values are distributions. 3. Explicit treatment of pollutant concentrations in various environmental media. 4. Mass balance model.	1. Does not allow spatial tracking of a pollutant. 2. Limited number of chemical species for which the model is applicable. 3. Limited in the extent of the environmental settings for which it can be applied.
HAPEM4 (inhalation)	1. Most input parameters are probabilistic. 2. Model can use both measured air quality data and modeled data from the ASPEN model or from air dispersion models. 3. Can model population exposures down to the census tract-level. 4. User can easily specify different demographic groups (providing they have data for the groups). 5. User can specify a "lag" factor for calculating indoor concentrations from pollutants penetrating from outside.	1. Single exposure route (inhalation) only. 2. The sequence of exposure events for activities is not preserved. 3. Does not provide any estimate of ventilation rate or delivered dose. 4. Currently, does not account for exposures to passive smoking.

[3] This table only includes models and modeling systems that are currently publicly available. OAQPS will continue to monitor and incorporate into TRIM.Expo, where appropriate, features, algorithms, and/or models that are under development. This includes ongoing work by the U.S. EPA on models and modeling systems, such as MENTOR and SHEDS.

Model	Strengths	Weaknesses
IEM (multimedia)	1. Establishes procedures for estimating the indirect human exposures and health risks that can result from the transfer of air pollutants to soil, vegetation, and water bodies. 2. Addresses exposures via multiple routes (inhalation, food, water, and soil ingestion, and dermal contact). 3. Has undergone extensive scientific review. 4. Has been widely used in EPA screening-level risk assessments. 5. Relatively simple spreadsheet model.	1. Based on annual average air concentrations and deposition rates. 2. Structured as a one-way process through a series of linked models. Not a truly coupled multimedia model. Does not have the ability to model feedback loops between media or secondary emissions. 3. Not designed to readily address spatial variability in exposures. 4. Not designed for probabilistic variability and uncertainty analysis. 5. Not suitable for estimating population exposures. 6. Does not provide a detailed time series of media concentrations or the resulting exposures. 7. Can only be applied to chemicals that are emitted into the air.
ISMCM (multimedia)	1. Considers all media, biological and non-biological, in one integrated system. 2. Includes both spatial and compartmental modules to account for complex transport of pollutants through the ecosystem. 3. Mass conserving model. 4. Includes estimation of intermedia transfer factors.	1. Links and spatial compartments are predetermined. 2. Not structured to incorporate uncertainty/variability directly into the model operation.
SCREAM2 (multimedia)	1. Can calculate indoor pollutant concentrations using the Indoor Air Quality Model (IAQM) or by using indoor/outdoor ratios. 2. Multipathway: inhalation, ingestion, and dermal. 3. Results reported in terms of both concentrations/dosages and risks. 4. Includes air dispersion algorithms to calculate air concentrations from emissions.	1. Deterministic. 2. Results reported for annual average exposures only.

Table B-3
Model Features for pNEM/CO

Attribute	Component	Remarks
General	Model name	pNEM/CO
	Pollutants of concern	Carbon monoxide
	Reference	Johnson et al. 1999. for U.S. EPA, OAQPS. Estimation of Carbon Monoxide Exposures and Associated Carboxyhemoglobin Levels in Denver Residents Using pNEM/CO (Version 2.0).
	Model status	Operates on either mainframe or PC. Further enhancements are currently ongoing.
	Contact/Affiliation	Harvey Richmond (U.S. EPA, OAQPS) (919) 541-5271
	Stochastic?	Yes – most variables chosen stochastically.
	Variability?	Yes – year-long exposure-event sequences (EES) use data from multiple subjects to better represent the variability of exposure that is expected to occur among the persons included in the cohort.
	Uncertainty?	Yes
Modeled area, study population, and modeling period	Study areas where model has been applied	Most recently to Denver. Application to Los Angeles is planned.
	Spatial designation of study area	50 km radius surrounding the city center of Denver.
	Sub-area designations	Six exposure districts, each 10 km in radius, surrounding fixed site CO monitors.
	Exposure duration for modeling	Typically one year.
	General population of interest	Typically defined as people with specific demographic or health status characteristics (*e.g.*, adults with ischemic heart disease).
	Special subgroups or designations	Demographic groups (DG): 1. Children 0 to 17 years; 2. Males, 18 to 44, working; 3. Males, 18 to 44, non-working; 4. Males 45 to 64, working; 5. Males 45 to 64, non-working; 6. Males 65+; 7. Females, 18 to 44, working; 8. Females, 18 to 44, non-working; 9. Females 45 to 64, working; 10. Females 45 to 64, non-working; 11. Females 65+
	Special attributes for subgroups	Each DG further subdivided into cohorts identified as a distinct combination of (1) home district, (2) demographic group, (3) work district (if applicable), (4) residential cooking fuel, and (5) replicate number.

Attribute	Component	Remarks
	Source of demographic data for study population	1990 Bureau of the Census.
Exposure events	Environmental media	Ambient air.
	Exposure media	Indoor air, outdoor air.
	Pathways	Ambient air and indoor air to personal air.
	Routes	Inhalation.
	Time resolution of exposure events	Inhalation: One minute. Ingestion: N/A
	Integration of exposures across multiple media	N/A.
	Method for determining pollutant contact rate	Inhalation: Ventilation rate (V_E) value estimated for each exposure-event. V_E expressed as liters of air respired per minute (liters min^{-1}). Ingestion: N/A.
	Activity pattern methodology	In typical pNEM applications, the EESs are determined by assembling activity diary records relating to individual 24-hour periods into a year-long series of records. Each exposure event within an EES was defined by (1) district, (2) CHAD location descriptor, (3) microenvironment, (4) CHAD activity descriptor, and (5) passive smoking status.
	Source of activity pattern data	Comprehensive Human Activity Database (CHAD).
	Time resolution of activity patterns	One minute.
	Microenvironments (Inhalation)	1. Indoors – residence 2 - 6. Indoors – nonresidence A - E 7. Indoors – residential garage 8. Outdoors – near roadway 9. Outdoors – other locations 10. Vehicle – automobile 11. Vehicle – other 12. Outdoors – public parking or fueling.
	Exposure locations (Ingestion)	N/A.
	Model calculates exposure of commuters	Yes – the number of commuters in each working cohort is calculated based on census data. In vehicle concentrations are estimated using a mass balance model (see Concentrations and Sources).
Concentrations and sources	Outdoor concentration determination method	Hourly-average CO concentrations for outdoor microenvironments based on data from fixed-site monitor and statistical relationship between fixed-site data and personal monitoring for outdoor microenvironments from a previous personal exposure study in Denver. Exposure districts are defined by monitor locations.

Attribute	Component	Remarks
	Indoor concentration determination method	Mass balance model used to estimate CO concentrations when a cohort is assigned to an indoor or motor vehicle microenvironment.
	In-vehicle concentration estimation	Mass balance model which accounts for outdoor concentration, air exchange rate, and passive smoking status of occupants.
	Passive smoking	CO contribution from indoor and in-vehicle passive smoking is modeled using a mass balance model.
	Other indoor sources	Gas stoves.
Extrapolation to study population	Method of allocating estimated exposures to study population	Entire population is simulated through the use of cohorts and census data relating cohorts to study area population.

Table B–4
Model Features for CalTOX

Attribute	Component	Remarks
General	Model name	CalTOX (California Total Exposure Model for Hazardous Waste Sites).
	Pollutants of concern	Potential toxic chemicals placed in landfills and in controlled and formerly uncontrolled hazardous waste sites. Chemicals on the Toxic Release Inventory (TRI) list emitted to air or water.
	References	McKone, T.E. 1993. CalTOX, A Multimedia Total-Exposure Model for Hazardous Wastes Sites. Lawrence Livermore National Laboratory, Livermore, CA, UCRL-CR-111456. Part I: Executive Summary; Part II: The Dynamic Multimedia Transport and Transformation Model; Part III: The Multiple-Pathway Exposure Model.
	Model status	Two versions of CalTOX are currently available from Cal-EPA: the original version developed for soil clean-up goals and a second version used for waste classification. A third version has been developed for use with the Environmental Defense Fund (EDF) Scorecard project.
	Contact/Affiliation	Tom McKone, Lawrence Berkeley National Laboratory (510-642-8771). Cal-EPA version: Ned Butler (916-323-3751).
	Stochastic?	Yes — all model inputs are represented by a mean value, coefficient of variability, and default distribution.
	Variability?	Yes — variability in exposure factors and in landscape factors are explicitly represented by probability distributions.
	Uncertainty?	Yes — all chemical-specific property data are represented by probability distributions.
Modeled area, study population, and modeling period	Study areas where model has been applied	For setting soil clean-up goals and for assessing residual risk at municipal landfills, CalTOX was used to represent the variability among all California land areas. For the EDF Scorecard project, CalTOX was used to represent the fate of air and water emissions in all 48 conterminous U.S. states.
	Spatial designation of study area	The designated study area is the environment impacted by either a waste site, air emissions, or water releases. 5,000 GIS land units were used to establish variability among California locations. For the EDF version, county-level climate and land data are used to establish state-level variability.
	Sub-area designations	The exposure location can be modeled with a residential, agricultural, commercial, or industrial scenario.
	Exposure duration for modeling	Exposure duration is variable depending on how long the exposure individual remains at the exposure location. Values as long as 70 years can be used.
	General population of interest	Populations in the landscape impacted by a waste site, air release, or water release.

Attribute	Component	Remarks
	Special subgroups or designations	Residential populations: Children (0 to 12 years) Adults (12 to 70 years). Agricultural populations. Those working or shopping at a commercial site. Those working at an industrial site.
	Special attributes for subgroups	Those with home gardens have been singled out for special attention.
	Source of demographic data for study population	EPA Exposure Factors Handbook.
Exposure events	Environmental media	Ambient air, surface soil, root zone soil, surface water and ground water.
	Exposure media	Indoor air; outdoor air; soil; house dust; tap water; food from home gardens and locally-produced fruits, vegetables, grains, fish, meat, milk, eggs; and dairy products.
	Pathways	Twenty-three pathways linking ambient media to exposure media.
	Routes	Inhalation, ingestion, dermal contact.
	Time resolution of exposure events	Inhalation: 1 day resolution to build the exposure scenario that is repeated over longer duration based on exposure frequency. Ingestion: 1 year. Dermal contact: 1 day resolution to build the exposure scenario that is repeated over a longer duration based on exposure frequency data.
	Integration of exposures across multiple media	Exposures are aggregated across all media and pathways to construct a total intake by route--inhalation, ingestion, and dermal contact.
	Method for determining pollutant contact rate	Inhalation: Activity adjusted breathing rate per unit body weight. Ingestion: Food consumption per unit body weight for each major food category is adjusted by fraction of food consumed within the contaminated landscape. Dermal contact: Activity data are used to establish long-term average rate and duration of contact with tap water and soil.
	Activity pattern methodology	For inhalation, the day is divided into the amount in each microenvironment and a breathing rate is assigned to each microenvironment. For ingestion, consumption of each major food category is divided into local and non-local sources. For dermal contact, the number and duration of water or soil contact events in a day are used.
	Source of activity pattern data	EPA Exposure Factors Handbook.

Attribute	Component	Remarks
	Time resolution of activity patterns	1 to 24 hours for inhalation. Annual consumption patterns for ingestion. Minutes to hours for dermal contact.
	Microenvironments (Inhalation)	Outdoors at home, Outdoors away from home, Indoors at home, Indoors in the bathroom.
	Exposure locations (Ingestion)	Residential environment.
	Model calculates exposure of commuters	No
Concentrations and sources	Outdoor concentration determination method	Multimedia mass balance using a dynamic regional fugacity model. Sources to air, soil, and water are allowed.
	Indoor concentration determination method	Based on a simple penetration model for outdoor air, a dust tracking model for soil pollutants, a transfer model for soil gas drawn into home, and a transfer model from water to indoor air.
	In-vehicle concentration estimation	Not explicitly represented; assumed to be equal to outdoor concentration.
	Passive smoking	Not included.
	Other indoor sources	Stripping of chemicals. Household water uses. Tracking of soil to house. Transfer of volatile chemicals from soil gas below homes.
Extrapolation to study population	Method of allocating estimated exposures to study population	Entire population is simulated through the use of probability distributions to represent variability and uncertainty in source-to-dose relationships.

Table B-5
Model Features for HAPEM4

Attribute	Component	Remarks
General	Model name	HAPEM4 (Hazardous Air Pollutant Exposure Model)
	Pollutants of concern	Criteria pollutants for which measured data, or HAPs for which modeled data can be obtained. Most recent application was for benzene.
	Reference	
	Model status	Operates on UNIX workstations.
	Contact/Affiliation	Ted Palma (U.S. EPA, OAQPS) (919) 541-5470
	Stochastic?	Yes – most variables chosen stochastically.
	Variability?	Yes – distributions available for many input variables.
	Uncertainty?	Not explicitely handled by the current model.
Modeled area, study population, and modeling period	Study areas where model has been applied	Most recently Houston and Phoenix. *Note – HAPEM4 may also be run in a *measured data mode* using data from fixed-site monitors. In this mode, the spatial designation and study areas are similiar to those in pNEM.
	Spatial designation of study area	Houston and Phoenix Metropolitan Statistical Areas (MSAs). *In measured data mode: study areas are typically a circle with a predetermined radius surrounding the city center.
	Sub-area designations	Census tracts. *In measured data mode: up to 18 exposure districts surrounding fixed-site monitors can be chosen for each MSA.
	Exposure duration for modeling	Typically one year (results are currently aggregated and reported as 3 month “seasons”).
	General population of interest	Typically defined as all persons described by the demographic groups for each sub-area designation.

Attribute	Component	Remarks
	Special subgroups or designations	Demographic groups (DG) in latest version (other groups for which census data are available may be input by the user): 1. Caucasians; 2. African-Americans; 3. All people not in DG 1 or 2; 4. Children 0 to 5 years; 5. Children 6 to 11 years; 6. Children 12 to 17 years; 7. Males 18 to 64; 8. Females 18 to 64; 9. Males 65+; 10. Females 65+; 11. People with gas stoves at home; 12. People without gas stoves at home; 13. People with attached garages at home; 14. People without attached garages at home; 15. People age 18 and older who work and were outdoors for at least 240 minutes (4 hrs) on the day recorded; 16. All persons.
	Special attributes for subgroups	No further sub-designations of population for this application. However, in future development, cohorts may be identified for commuting by specifying a home district and work district. Other cohort attributes may also be specified in future versions.
	Source of demographic data for study population	1990 Bureau of the Census.
Exposure events	Environmental media	Ambient air.
	Exposure media	Indoor air and outdoor air.
	Pathways	Ambient air and indoor air to personal air.
	Routes	Inhalation.
	Time resolution of exposure events	Inhalation: 1 to 60 minutes; obtained from CHAD. Ingestion: N/A.
	Integration of exposures across multiple media	N/A.
	Method for determining pollutant contact rate	Inhalation: N/A. Ingestion: N/A.

Attribute	Component	Remarks
	Activity pattern methodology	Information on the time spent in various microenvironments (μe) for each individual are used. * Note, this is not an activity sequence, rather it is the total time spent in each μe during each 1-hour block of time throughout the day. A daily record (comprised of 24 separate hours) is chosen using the Monte Carlo technique. The record chosen is matched to the day being modeled by using the maximum outdoor temperature for each hour. The number of minutes spent in a particular μe for each individual selected and for each hour of the day are calculated. The exposures reported for each DG are the averages of all individuals sampled from each group.
	Source of activity pattern data	Comphrensive Human Activity Database (CHAD).
	Time resolution of activity patterns	1 to 60 minutes.
	Microenvironments (Inhalation)	1. In vehicle – car 2. In vehicle – bus 3. In vehicle – truck 4. In vehicle – other 5. Indoors – public garage 6. Outdoors – parking lot/garage 7. Outdoors – near a road 8. Outdoors – motorcycle 9. Indoors – service station 10. Outdoors – service station 11. Indoors – residential garage 12. Indoors – other repair shop 13. Indoors – residence, no inside sources of CO 14. Indoors – residence, gas stove present 15. Indoors – residence with attached garage 16. Indoors – residence with stove and attached garage 17. Indoors – office 18. Indoors – store 19. Indoors – restaurant 20. Indoors – manufacturing facility 21. Indoors – school 22. Indoors – church 23. Indoors – shopping mall 24. Indoors – auditorium 25. Indoors – health care facility 26. Indoors – other public building 27. Indoors – other location 28. Indoors – not specified 29. Outdoors – construction site 30. Outdoors – residential grounds 31. Outdoors – school grounds 32. Outdoors – sports arena 33. Outdoors – park/golf course 34. Outdoors – other location 35. Outdoors – not specified 36. In vehicle – train/subway 37. In vehicle – airplane.
	Exposure locations (Ingestion)	N/A.

Attribute	Component	Remarks
	Model calculates exposure of commuters	Yes – commuting patterns of workers between exposure districts are modeled. The "travel time to work" data from the 1990 census are used to develop the commuting patterns. A program uses this to build an array of probabilities of the movement of working commuters for each census tract-to-tract combination.
Concentrations and sources	Outdoor concentration determination method	*Modeled air quality mode:* The model is currently configured to read output at the census tract-level from the ASPEN (Assessment System for Population Exposure Nationwide) model. *Measured data mode:* Hourly-average CO concentrations taken from fixed-site monitors. Exposure districts defined by monitor locations.
	Indoor concentration determination method	Uses microenvironmental factors. These factors are obtained from field studies through a linear regression of microenvironmental concentrations against fixed-site monitoring concentrations.
	In-vehicle concentration estimation	Microenvironmental factor (same as indoor concentration determination method above).
	Passive smoking	N/A.
	Other indoor sources	Gas stoves and residences with attached garages through the use of additive factors (user supplied).
Extrapolation to study population	Method of allocating estimated exposures to study population	Entire population is simulated through the use of cohorts and census data relating cohorts to study area population.

Table B–6
Model Features for SCREAM2

Attribute	Component	Remarks
General	Model name	SCREAM2 (South Coast Risk and Exposure Model, Version 2.0).
	Pollutants of concern	HAPs for which emissions data can be obtained.
	Reference	Rosenbaum, A.S. User's Guide for an Enhanced Version of the South Coast Air Quality Management District's Air Toxics Risk and Exposure Assessment Model (SCREAM2 – PC version).
	Model status	Operates on UNIX workstations and PCs.
	Contact/Affiliation	Unix: Henry Hogo, South Coast Air Quality Management District, (909) 396-3100. PC: Arlene Rosenbaum, ICF Consulting Group, (415) 507-7192.
	Stochastic?	No.
	Variability?	No.
	Uncertainty?	No.
Modeled area, study population, and modeling period	Study areas where model has been applied	California's South Coast Air Basin.
	Spatial designation of study area	All block groups in the South Coast Air Basin as defined by the Bureau of the Census.
	Sub-area designations	Block group centroids.
	Exposure duration for modeling	One year.
	General population of interest	Typically defined as all persons described by the demographic groups for each sub-area designation.
	Special subgroups or designations	Default demographic groups (other groups for which census data are available may be input by the user): 1. Students 18 and over; 2. Managers and professionals; 3. Sales workers; 4. Clerical and kindred workers; 5. Craftsmen and kindred workers; 6. Farmers; 7. Operatives and laborers; 8. Service, military, and private household workers; 9. Housepersons; 10. Unemployed and retired persons; 11. Children under 5; 12. Children 5 to 17.
	Special attributes for subgroups	Each demographic group is further sub-divided into cohorts identified as a distinct combination of (1) home district, (2) demographic group, and (3) work district (if applicable),

Attribute	Component	Remarks
	Source of demographic data for study population	1990 Bureau of the Census and Southern California Association of Governments (commuting).
Exposure events	Environmental media	Ambient air, soil, surface water, food crops.
	Exposure media	Indoor air, outdoor air, soil ingested or contacted, drinking water, food ingested, and breast milk.
	Pathways	Ambient air; indoor air to personal air; soil to ingested soil, contacted soil; soil to root crops and leafy crops to ingested food; soil and surface water to animal food sources to ingested food; ambient air and soil to surface water to drinking water; ingested food and drinking water to ingested breast milk.
	Routes	Inhalation, ingestion, dermal contact.
	Time resolution of exposure events	Inhalation: 1 hour. Ingestion: daily.
	Integration of exposures across multiple media	Yes.
	Method for determining pollutant contact rate	Inhalation: N/A. Ingestion: N/A.
	Activity pattern methodology	Information on the fraction of time spent in various microenvironments by each demographic group for each of 24 hours is used.
	Source of activity pattern data	Roddin, Ellis, and Siddiqee (1979) "Background Data for Human Activity Patterns, Vols. I and II." SRI International.
	Time resolution of activity patterns	1 hour.
	Microenvironments (Inhalation)	1. Indoors – residence 2a. Indoors – office 2b. Indoors – school 3. In vehicle 4. Outdoors – near a road 5. Outdoors – other location.
	Exposure locations (Ingestion)	Home
	Model calculates exposure of commuters	Yes – commuting patterns of workers between exposure districts are modeled. Commuting data provided by the Southern California Association of Governments.
Concentrations and sources	Outdoor concentration determination method	Estimated from data on emission sources with the air dispersion module.
	Indoor concentration determination method	Alternative 1: the Indoor Air Quality Model (IAQM), a mass balance model using outdoor concentration, air exchange rates, filtration rates, and mixing ratios. Alternative 2: indoor/outdoor concentration ratios obtained from field studies.
	In-vehicle concentration estimation	Same as for indoor concentration determination method.
	Passive smoking	N/A.
	Other indoor sources	Additive factors (user supplied).

Attribute	Component	Remarks
Extrapolation to study population	Method of allocating estimated exposures to study population	Entire population is simulated through the use of cohorts and census data relating cohorts to study area population.

Table B–7
Model Features for CPIEM

Attribute	Component	Remarks
General	Model name	CPIEM (California Population Indoor Exposure Model)
	Pollutants of concern	Benzene, benzo[a]pyrene, CO, chloroform, formaldehyde, NO_2, PM_{10}, perchloroethylene, trichloroethylene, and PAHs. User has the ability to input data for other chemicals.
	Reference	California Air Resources Board. 1998. Development of a model for assessing indoor exposure to air pollutants. Sacramento, CA. Report No. A933-157. January 1998.
	Model status	Operates on PCs.
	Contact/Affiliation	Susan Lum (California Air Resources Board) (916) 323-5043
	Stochastic?	Yes.
	Variability?	Yes.
	Uncertainty?	The model needs to be run several times with all inputs the same except the random number seed. Variance in each output parameter across the repeated model runs is then used to characterize the uncertainty through a measure such as the coefficient of variation.
Modeled area, study population, and modeling period	Study areas where model has been applied	Most recently applied to the South Coast region (encompasses Los Angeles and surrounding areas).
	Spatial designation of study area	South Coast region, San Francisco Bay area, or the remainder of the State of California.
	Sub-area designations	County.
	Exposure duration for modeling	Varies (user-defined).
	General population of interest	California population.
	Special subgroups or designations	Certain identified subgroups of the population such as individuals who may be sensitive to indoor pollutants.
	Special attributes for subgroups	For purposes of calculating potential dose, the population was further segregated into the following groups: adult males, adult females, and children (age 12 and younger).
	Source of demographic data for study population	
Exposure events	Environmental media	Indoor air and outdoor air.
	Exposure media	Indoor air and outdoor air.
	Pathways	Ambient air and indoor air to personal air.
	Routes	Inhalation

Attribute	Component	Remarks
	Time resolution of exposure events	Inhalation: 1-hour periods; but these may be aggregated into an 8-hour exposure event. Also, a 12- or 24-hour exposure event may be specified (the basis for these are a single activity per individual). Ingestion: N/A.
	Integration of exposures across multiple media	N/A.
	Method for determining pollutant contact rate	Inhalation: Breathing rates are supplied by the model for three age/sex groups (adult males, adult females, and children under age 12) and four activity levels (resting, light, moderate, heavy). Using information sampled on the quantity of time spent in an environment and the concentration in each environment, combined with the breathing rates, the model calculates the potential inhaled dose received by each individual in each environment. Ingestion: N/A.
	Activity pattern methodology	Location codes were grouped into nine types of environments. Then, the time spent was summed across locations within each environment type. This was done separately for each individual for a 24-hour period, 12-hour daytime and nighttime periods, 24 sequential 1-hour periods, and 24 running 8-hour periods. Within each of the nine environment types, each individual's time was further disaggregated according to four activity levels (resting, light, moderate, heavy). In addition, demographic information (*e.g.*, age, gender, location of residence, month and day of week when the activity was recorded, work status, income) on each person was matched to their location/activity information. An index number was assigned sequentially to each record of each file in order to enable linking the information.
	Source of activity pattern data	Two ARB-sponsored studies: The first for a target population of adults (18 years and older) and adolescents (12 to 17 years), provided 1,762 profiles; the second, for a target population of children (aged 11 years and younger), provided 1,200 profiles.
	Time resolution of activity patterns	One minute.
	Microenvironments (Inhalation)	Environment types: residences (numerous microenvironments); offices (office, bank, or post office); industrial plants; school; travel in enclosed vehicles (several microenvironments); stores and other public buildings (several microenvironments); restaurants and lounges; other indoor locations (several microenvironments); outdoors (several microenvironments).
	Exposure locations (Ingestion)	N/A.
	Model calculates exposure of commuters	Distributional data on concentrations for travel in enclosed vehicles were taken from studies identified in the literature.

Attribute	Component	Remarks
Concentrations and sources	Outdoor concentration determination method	Two options are provided for inputting outdoor concentrations: daily-average values and hourly-average values. Sources of data identified for input (for formaldehyde, several VOCs, B(a)P, PM_{10}, NO_2, and CO) include state/local ambient air monitoring networks and some indoor air monitoring studies where outdoor concentrations were measured in conjunction with indoor measurements.
	Indoor concentration determination method	Mass balance model. Each source is associated with both a pollutant (a source may be associated with more than one pollutant) and a source category (long-term, episodic, or frequent). For each source category, different input parameters are required by the model which are sampled from distributions. The model calculates the initial indoor concentration and the hourly emission rates. These contributions are then used by the mass balance routine to calculate the indoor concentrations.
	In-vehicle concentration estimation	Distributional data on concentrations for travel in enclosed vehicles were taken from studies identified in the literature.
	Passive smoking	
	Other indoor sources	Examples of the indoor sources considered for pollutants provided with the model are tobacco smoking, unburned natural gas (leaks), various consumer products, wood burning, range cooking, range pilot light, chlorinated water supply, pressed wood products, vacuuming/sweeping, and dry-cleaned clothes. **Note– Data are not available for each pollutant being emitted from each of these identified sources.*
Extrapolation to study population	Method of allocating estimated exposures to study population	

Table B–8
Model Features for SHEDS

Attribute	Component	Remarks
General	Model name	SHEDS (Stochastic Human Exposure and Dose Simulation) Model
	Pollutants of concern	pesticides, particulate matter, and other POPs, metals, and air toxics
	References	Zartarian V.G., Özkaynak H., Burke J.M., Zufall M.J., Rigas M.L., and Furtaw Jr. E.J. A Modeling Framework For Estimating Children's Residential Exposure and Dose to Chlorpyrifos Via Dermal Residue Contact and Non-Dietary Ingestion. Submitted to Environmental Health Perspectives. September 1999. Özkaynak H., Zufall, M., Burke, J., Xue, J., Zidek, J. 1999a. Predicting population exposures to PM10 and PM2.5. Presented at PM Colloquium, Durham, NC. June, 1999. Özkaynak H., Zufall, M., Burke, J., Xue, J., Zidek, J. 1999b. A Probabilistic Population Exposure Model for PM10 and PM2.5. Presented at 9th Conference of the International Society of Exposure Analysis, Athens, Greece. September 5-8, 1999.
	Model status	Prototype first-generation SHEDS-Pesticides model has been developed. A case study for children and chlorpyrifos has been conducted using 1-stage Monte Carlo sampling. Currently case study is being completed for 2-stage Monte Carlo sampling to conduct variability and uncertainty analyses. Next generation will focus on pesticides and other multimedia, multipathway pollutant for different population cohorts, and will assess both cumulative and aggregate dose. Prototype first-generation SHEDS-PM model has been developed. A PM10 case study for Vancouver, Canada has been conducted using 1-stage Monte Carlo sampling. Subsequent generations will focus on modeling both PM10 and PM2.5 exposure and dose in a selected U.S. city, using 2-stage Monte Carlo sampling.
	Contact/Affiliation	Halûk Özkaynak, U.S. EPA National Exposure Research Laboratory (919-541-5172) Valerie Zartarian (SHEDS-Pesticides), U.S. EPA National Exposure Research Laboratory (703-648-5538) Janet Burke (SHEDS-PM), U.S. EPA National Exposure Research Laboratory (919-541-0820) Maria Zufall (SHEDS-PM), U.S. EPA National Exposure Research Laboratory (919-541-5461)
	Stochastic?	Yes - all model inputs are represented by a probability distribution

Attribute	Component	Remarks
	Variability?	Yes - variability of inputs is explicitly represented by user-specified probability distributions and Monte Carlo sampling is applied to quantify variability in model outputs.
	Uncertainty?	Yes - for each input parameter probability distribution, associated uncertainty distributions can also be specified. 2-stage Monte Carlo sampling is applied to analyze uncertainty in model outputs.
Modeled area, study population, and modeling period	Study areas where model has been applied	First-generation SHEDS-Pesticides model has been applied to estimate children's indoor and outdoor (home lawn) exposures and doses to chlorpyrifos. Children were sampled from the National Human Activity Pattern Survey, which includes all 48 conterminous U.S. states. First-generation SHEDS-PM model has been applied to estimate PM10 exposures to individuals in Vancouver, Canada.
	Spatial designation of study area	The designated study area is the geographic location associated with the user-specified cohort from national time/location/activity surveys in EPA's Consolidated Human Activity Database (CHAD).
	Sub-area designations	Sub-area designations are the set of locations (microenvironments) occupied by individuals sampled from the time/location/activity pattern surveys in EPA's Consolidated Human Activity Database (CHAD).
	Exposure duration for modeling	Daily exposure and dose profiles are modeled for each individual. The time scales used to generate these profiles differ by route. For inhalation, the time scale ranges from 1 minute to 12 hours, depending on the pollutant and diary selected. For dermal contact and non-dietary ingestion, the time scale is 5 seconds. For dietary ingestion, the time scale for ingestion is instantaneous for each eating/drinking event, but absorption is calculated on a 30-minute time scale after each ingestion event. The daily profiles correspond to time periods associated with the user-specified environmental concentrations (*e.g.*, <1 day, 1-7 days, 8-30 days, 30-365 days post-pesticide application).
	General population of interest	The U.S. population as represented by individuals in time/location/activity surveys contained in EPA's Consolidated Human Activity Database (CHAD).
	Special subgroups or designations	The first generation of SHEDS-Pesticides focuses on residential exposures to children (0-4 years and 5-9 years). The next generation will be able to address residential, non-residential, and occupational exposures for other cohorts of interest. The first generation of SHEDS-PM estimates exposures by gender and age category.
	Special attributes for subgroups	The first generation of SHEDS-Pesticides focuses on children living in residences with lawns.
	Source of demographic data for study population	Time/location/activity surveys in EPA's CHAD.

Attribute	Component	Remarks
Exposure events	Environmental media	SHEDS is a concentration-to-dose model in which the user enters distributions for residues or concentrations in exposure media rather than environmental media (except for ambient air and surface soil).
	Exposure media	indoor air; outdoor air; commuting/in-vehicle air; soil; house dust; surface residues (indoor and lawn); hand and object residues; tap water; food and beverages
	Pathways	Ingestion of residues in food and beverages by eating/drinking event; Dermal contact with soil, dust, or residues on surfaces; Non-dietary ingestion of residues on skin and objects mouthed; Inhalation of pollutants in indoor, outdoor, and commuting/in-vehicle locations
	Routes	Inhalation, Dietary Ingestion (food, drinking water, other beverages), Non-Dietary Ingestion (hand-to-mouth and object-to-mouth), Dermal Contact
	Time resolution of exposure events	Inhalation: Daily profiles with down to 1 minute resolution. Dermal and Non-Dietary Ingestion: Daily profiles with 5-second resolution. Dietary Ingestion: Daily profiles with 30-minute resolution for absorption; residues ingested by eating events assumed to be instantaneous.
	Integration of exposures across multiple media	Exposures are estimated for each route and pathway via sequential exposure profiles. Corresponding dose profiles for each route and pathway are calculated then summed across routes.
	Method for determining pollutant contact rate	Inhalation: For sampled individual's daily sequential time/location/activity diary events, combine location-specific air concentrations (drawn from input probability distributions), activity-specific inhalation rates (in CHAD, derived using METS), and inhalation absorption fraction.
		Dietary Ingestion: For sampled individual's daily sequential time/location/activity diary events, combine total residue mass ingested during each eating/drinking event (sampled from measured or modeled distributions) with dietary absorption fraction.
		Dermal Contact: For sampled individual's daily sequential time/location/activity diary events, simulate sequences of microlevel object contact events using probabilities developed from videography study data. For each discrete microlevel contact event, combine surface residue, transfer or removal efficiency, and dermal or GI absorption rate constant.

Attribute	Component	Remarks
	Activity pattern methodology	Daily time/location/activity profiles are obtained from surveys contained in EPA's CHAD (*e.g.*, NHAPS, CARB, U. Michigan). For inhalation, the day is divided into 1-minute to 12 hour sequential activities (depending on the pollutant and diary selected). For ingestion, the day is divided into 30-minute sequential macro-activities and eating/drinking events. For dermal and non-dietary ingestion, the day is divided first into 30-minute sequential macro-activities, then each macro-activity is divided into 5-second contact events. Daily activity pattern time profiles for each route are combined with concentrations, exposure factors, and dose factors to yield daily exposure and dose profiles.
	Source of activity pattern data	For macrolevel activity patterns, time/location/activity surveys contained in EPA's CHAD (*e.g.*, NHAPS, CARB, U. Michigan) are used. For microlevel activity patterns, data on contact frequency and duration for different body parts and surfaces are obtained from available videography studies.
	Time resolution of activity patterns	Inhalation: 1 minute to 12 hours, depending on the pollutant and diary selected.. Dietary ingestion: Daily consumption patterns, with instantaneous ingestion assumed for each eating/drinking event, and 30-minute time steps for GI absorption. Dermal and non-dietary ingestion: 5-second time steps for contact events occurring within each macro-activity.
	Microenvironments (Inhalation)	In the first-generation of SHEDS: indoors at home and outdoors at home, non-residential locations (SHEDS-PM), and in vehicles (SHEDS-PM)
	Exposure locations (Ingestion)	Microenvironments in time/location/activity surveys in which sampled individuals ingest food or beverages.
	Model calculates exposure of commuters	First generation of SHEDS calculates in-vehicle exposures, but does not explicitly incorporate pollution gradients during commuting. Next generation will include air concentrations in specified cohort's commuting area.
Concentrations and sources	Outdoor concentration determination method	SHEDS requires user to enter distributions for concentrations in exposure media. Distributions for outdoor concentrations can be derived from measurements or from fate and transport models.
	Indoor concentration determination method	SHEDS-Pesticides requires user to enter distributions for concentrations in exposure media. Distributions for indoor concentrations can be derived from measurements or from fate and transport models. SHEDS-PM uses a physical or empirical mass balance model to estimate indoor concentrations.
	In-vehicle concentration estimation	SHEDS requires user to enter distributions for concentrations in exposure media. In-vehicle air concentrations are modeled using available measurements.
	Passive smoking	Indoor PM passive smoking concentrations are modeled using a mass balance model.

Attribute	Component	Remarks
	Other indoor sources	Other indoor sources (*e.g.*, tracked-in soil, stripping of chemicals via household water use, pesticide application rates) are not explicitly included in SHEDS-Pesticides, but are implicitly included through user-specified concentrations for indoor air and surfaces. SHEDS-PM includes cooking and resuspension as other indoor sources of particles.
Extrapolation to study population	Method of allocating estimated exposures to study population	Daily exposures and doses are simulated for individuals in the specified cohort by combining actual macro-level and micro-level activity data with residues or concentrations in exposure media and exposure and dose factors. 2-stage Monte Carlo sampling is applied to simulate population distributions.

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